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Next Generation Nuclear Plant–
Design Methods Development and Validation Research and Development Program Plan

Idaho National Engineering and Environmental Laboratory

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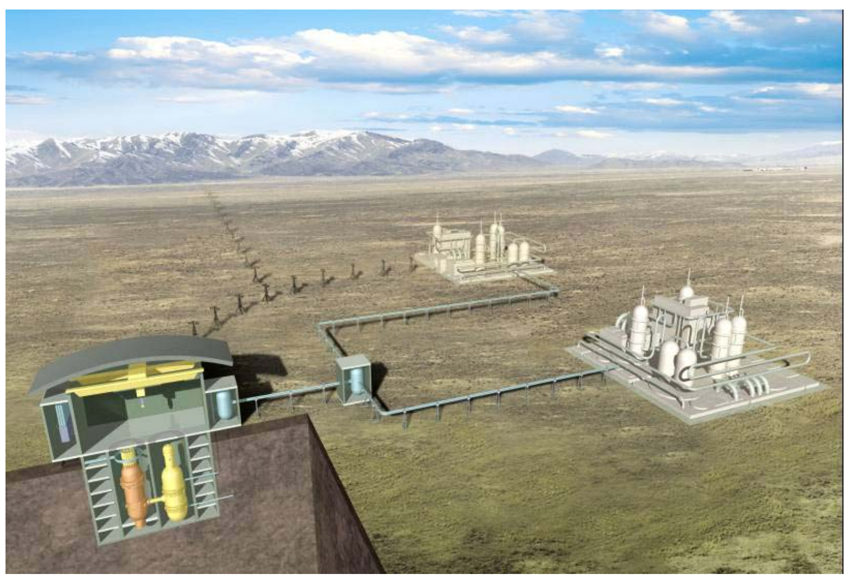

Next Generation Nuclear Plant (NGNP)

Idaho National Engineering and Environmental Laboratory
Bechtel BWXT Idaho, LLC

INEEL/EXT-04-02293

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Design Methods Development and Validation
Research and Development Program Plan

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This is to acknowledge that I served as external reviewer for the report entitled "Next Generation Nuclear Plant – Design Methods Development and Validation Research & Development Program Plan, INEEL/EXT-04-02293, Rev 0, Idaho National Engineering and Environmental Laboratory, September 2004," and believe that it has identified the R&D needs for NGNP reactor design methods.

Temitope A. Taiwo, Manager, Nuclear Systems Modeling, ANL

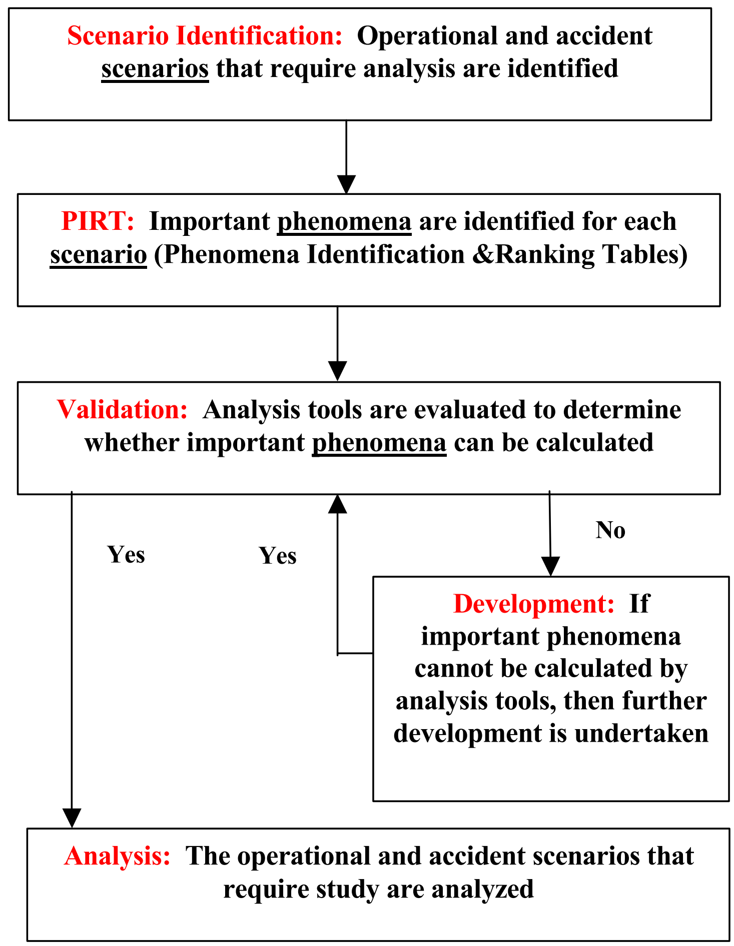
EXECUTIVE SUMMARY

One of the great challenges of studying, designing, and licensing the NGNP is the successful completion of the tasks that confirm that the intended NGNP analysis tools can be used with confidence to make decisions and to assure all that the reactor systems are safe and meet the performance objectives of the Generation IV Program. The research and development (R&D) projects outlined in this plan will ensure the tools used to perform the required calculations and analyses can be trusted. In other words, the task before us is to ensure the calculational envelope of the tools used to analyze the NGNP reactor systems encompasses, or is larger than, the operational and transient envelope of the NGNP itself.

This plan focuses on the development of tools to assess the neutronic and thermal-hydraulic behavior of the plant. The fuel behavior and fission product transport models are discussed in the Advanced Gas Reactor (AGR) program plan. Various stress analyses and mechanical design tools will also need to be developed and validated. Those tools will be addressed in a subsequent revision of this program plan.

The calculational envelope of the neutronics and thermal-hydraulic software tools intended to be used on the NGNP is defined by the scenarios and phenomena that these tools can calculate with confidence. Users of the software can only be confident when the results produced by the tools have been shown to produce reasonable agreement[a] with first-principle results, thought-problems, and data that describe the "highly-ranked" phenomena inherent to all operational conditions and the important accident scenarios for the NGNP.

The R&D process itself is outlined in the figure at right. The requirements associated with scenario identification, defining the phenomena identification and ranking tables (PIRT), completing the required development, and performing the necessary validation studies must all be completed prior to performing the required analyses confidently.



Research & development process

The NGNP design has not yet been selected. Consequently, the R&D process is focused on scenarios and "highly-ranked" phenomena that have been identified as important by the advanced gas-cooled reactor community, in the past, for the designs being considered as candidates for the very high temperature reactor (VHTR), the reactor component of the NGNP. This approach has

a. Reasonable agreement is achieved when the calculation generally lies within the uncertainty band of the data used for validation and always shows the same trends as the data. Code deficiencies are minor.

resulted in an NGNP-specific "first-cut" PIRT from which the R&D is being defined using the following assumptions:

- The selected NGNP design could be either a pebble-bed or a block-type reactor.

- For fiscal years 2004 and 2005 the highest priority R&D is aimed at properly calculating the thermal-hydraulic conditions in the hot channels and the mixing in the lower plenum during normal operation and the behavior of the plant during depressurized conduction cooldown (DCC) and pressurized conduction cooldown (PCC) accident scenarios.

- The calculational and experimental needs, and consequently the required R&D, will be focused in eight distinct areas based on the relative state of the software in each. The areas are:

  (i) Basic differential and integral nuclear cross-section data measurement & evaluation, including mathematically rigorous sensitivity studies of the effects of uncertainties in the differential nuclear data and other independent design variables on key integral reactor properties (the task of characterizing the nuclear fuel, fission products, moderator, and other relevant materials effect on the system reactivity, neutron flux distribution, and power production).

  (ii) Reactor assembly cross-section preparation (the task of translating the fundamental data, characterized in area (i), into formats and states useful for analysis).

  (iii) Discrete ordinates transport (the process of approximating the neutron flux in a tractable manner for analysis).

  (iv) Nodal diffusion (calculation of the energy and spatial flux profiles, reaction rates, reactivity changes, etc.).

  (v) Reactor kinetics (calculation of spatial changes in flux and power level as a function of time during postulated transients).

  (vi) (vi) Thermal-hydraulics (the models that describe the fluid behavior and heat transfer behavior during steady-state and transient conditions for the scenarios of interest).

  (vii) Fuel behavior.

  (viii) Fission product transport (determination of fission product movement once fission products have escaped from the confines of the fuel).

For now, the R&D described in this plan focuses on areas (i) through (vi). Fuel behavior and fission product transport will be addressed by other Generation IV programs. Based on the above, a set of broad R&D projects has been defined as outlined in the following table. Although the fiscal year 2005 will begin with funding levels awaiting resolution by Congress, the assumed funding level is: $2,619k considering carryover from fiscal year 2004.

The R&D projects tabulated below are ordered according to the region in the reactor [inlet and outlet plena, core, reactor cavity cooling system (RCCS), downcomer and vessel structure, containment, and overall system behavior] for the DCC, PCC, and rated operational conditions.

Summary of R&D Projects[a]: Planned for immediate future or ongoing.

Region of System	Operational Conditions	Depressurized Conduction Cooldown	Pressurized Conduction Cooldown
Inlet Plenum			*IP1: Validation of CFD mixing calculation during transient.*
Core	*CO1: Nuclear data measurements to reduce calculational uncertainty.* *CO2: Modification of cross-section generation code to treat low-energy resonances with upscattering. Development of improved method for computing Dancoff factors.* **CO3: Characterization of hot channel temperatures and fluid behavior at operational conditions.** *CO4: Validation using integral experimental data.* *CO5: Additional physics modeling code improvements.*	CD1: Validation of systems analysis codes to demonstrate capability to predict thermal behavior. *CD2: Validation of models that calculate fission product release from fuel.* *CD3: Validation and calculation of air ingress and potential water ingress behavior into reactor vessel and core region.*	CP1: Validation of systems analysis codes to demonstrate capability to predict thermal and hydraulic behavior.
Outlet Plenum	PO1: Validation of CFD mixing using mixed index refraction (MIR) facility data & data available in literature	*PD1: Validation of CFD mixing during operational transients and effect on turbine operational characteristics.*	*PP1: Validation of CFD mixing during operational transients and effect on turbine operational characteristics.*
RCCS	*RO1: Validation of natural convection characteristics in cavity at operational conditions.* *RO2: Characterization of natural convection characteristics in cavity at operational conditions.*	*RD1: Validation of heat transfer & convection cooling phenomena present in reactor cavity and via RCCS.*	*RP1: Validation of heat transfer & convection cooling phenomena present in reactor cavity and via RCCS.*
Turbine Inlet	*TO1: Validation of CFD mixing between outlet plenum and turbine inlet; effect of temperature variation on turbine blade thermal stresses*		
Downcomer & Vessel Structure		VD1: Validation of peak vessel wall temperatures as predicted using CFD.	VP1: Validation of peak vessel wall temperatures as predicted using CFD.
Containment		*ConD1: Validation of fission product transport, including dust, into containment and regions for potential release to environment.*	
System Behavior	SO1: Validation & calculation of system operational envelope—including turbine/compressor components.	SD1: Validation & calculation of reactor systems.	SP1: Validation & calculation of reactor systems.

a. **Bold black font = ongoing work**; normal font = some work completed but more proposed; *italic font = proposed work.*

CONTENTS

FIGURES

TABLES

ACRONYMS

AVR	Arbeitsgemeinschaft Versuchsreaktor
ANL	Argonne National Laboratory
BWR	boiling water reactor
CFD	computational fluid dynamics
CFR	Code of Federal Regulations
DCC	Depressurized conduction cooldown scenario
DOE	U. S. Department of Energy
FSAR	Final Safety Analysis Report
FTE	full-time equivalent
FY	fiscal year
GDC	General Design Criteria
GIF	Generation IV International Forum
GSI	Generic Safety Issue
GT-MHR	Gas Turbine-Modular Helium Reactor
GTHTR	Gas Turbine High Temperature Reactor
HENDEL	Helium Engineering Demonstration Loop
HTGR	High Temperature Gas Reactor
HTR-10	Chinese High Temperature Gas-Cooled Reactor
HTR	high-temperature reactor
HTTR	High Temperature Engineering Test Reactor
IHX	intermediate heat exchanger
INEEL	Idaho National Engineering and Environmental Laboratory
ITRG	Independent Technology Review Group
IPNS	Intense Pulsed Neutron Source
JAERI	Japan Atomic Energy Research Institute

LWR	light water reactor
LANSCE	Los Alamos Neutron Science Center
MWe	megawatts-electrical
MWt	megawatts-thermal
NGNP	Next Generation Nuclear Plant
NRC	U.S. Nuclear Regulatory Commission
PBR	Pebble-bed reactor
PBMR	Pebble-bed modular reactor
PMR	Prismatic modular reactor
PCC	Pressurized conduction cooldown scenario
PSAR	Preliminary Safety Analysis Report
PV	pressure vessel
PWR	Pressurized Water Reactor
RCCS	Reactor cavity cooling system
R&D	Research and Development
RPV	Reactor Pressure Vessel
TRISO	ceramic-coated-particle fuel
V&V	verification and validation

Next Generation Nuclear Plant – Design Methods Development and Validation Research and Development Program Plan

1. INTRODUCTION

In May 2004, the U.S. Department of Energy (DOE) released a "Request for Information and Expressions of Interest" (EOI) on the Next Generation Nuclear Plant (NGNP). The DOE objective: "… is to conduct research, development, and demonstration of a next-generation nuclear power reactor in order to establish advanced technology for the future production of safe, efficient, and environmentally-acceptable power and to demonstrate the economic and technical feasibility of such facilities to the U.S. electric power industry."

Although a rigorous schedule has not been defined yet, planning is aimed at starting the NGNP in approximately 2017. Prior to completing the final design, three intermediate steps will likely be taken: the preconceptual design between circa 2006 and 2007; the conceptual design between 2008 and 2009; and the preliminary design between 2010 and 2011. The final design was assumed to begin circa 2012. This unofficial schedule was used to govern the research and development (R&D) planning discussed herein. The software to be used to perform realistic calculations of the behavior of the NGNP during important operational conditions and various transients must be verified and validated (V&V) prior to application to the final design in 2012.

The process of demonstrating the NGNP will require rigorous analysis of the plant's projected behavior under all postulated operational and accident conditions such that the operational and accident envelopes for the NGNP are fully defined and understood. Thus, the analytical tools must be demonstrated to be capable of analyzing the plant's behavior in the plant's operational and accident envelopes.

R&D specific to the NGNP and conducted to date is based on the very high temperature reactor (VHTR) concept promulgated in the Generation IV technology roadmap (see Generation IV International Forum, 2002). Although the NGNP may or may not resemble this concept, early thinking on the most likely candidates for the NGNP has led researchers to consider the prismatic and pebble-bed variants of the very high temperature gas-cooled thermal reactor.[b] These designs have been demonstrated and have been studied extensively. Because some of their operational and accident characteristics have been identified in past studies, these characteristics are a good starting point for research and development (R&D) planning and studies.

This R&D plan focuses on the development of tools to assess the neutronic and thermal-hydraulic behavior of the plant. The fuel behavior and fission product transport models are discussed in the Advanced Gas Reactor (AGR) program plan. Various stress analyses and mechanical design tools will also need to be developed and validated. Those tools will be addressed in a subsequent revision of this program plan. This report only addresses R&D needs regarding neutronics and thermal-hydraulics specific to very high temperature gas-cooled thermal reactors.

The process of identifying R&D needs and then formulating plans is straightforward, although there are many unknowns and the process itself is iterative. The process is shown in flow chart form in

b. The Ft. St. Vrain power plant was a prismatic configuration (also called a block-type) reactor and the German Arbeitsgemeinschaft Versuchsreaktor (AVR) was a pebble-bed configuration reactor.

Figure 1. In essence it is a five stage process that consists of (i) identifying the scenarios of importance, (ii) identifying the key phenomena for the scenarios of importance, (iii) determining whether the tools to be used to analyze the scenario progressions are adequate, (iv) correcting or completing existing software and carrying out any software development that may be needed to ensure the analysis tools are adequate, and finally (v) performing the required analyses.

The remainder of this report is divided into seven sections. Section 2 describes the NGNP design concepts, including operating conditions and transients. Section 3 defines the methodology for producing validated analytical tools for the analysis of the NGNP. Sections 4, 5, and 6 detail the planned research program in the three key areas of Nuclear Data Measurements, Reactor Kinetics and Neutronics, and Thermal-Hydraulics, respectively. Section 7 summarizes the R&D. Section 8 presents the references.

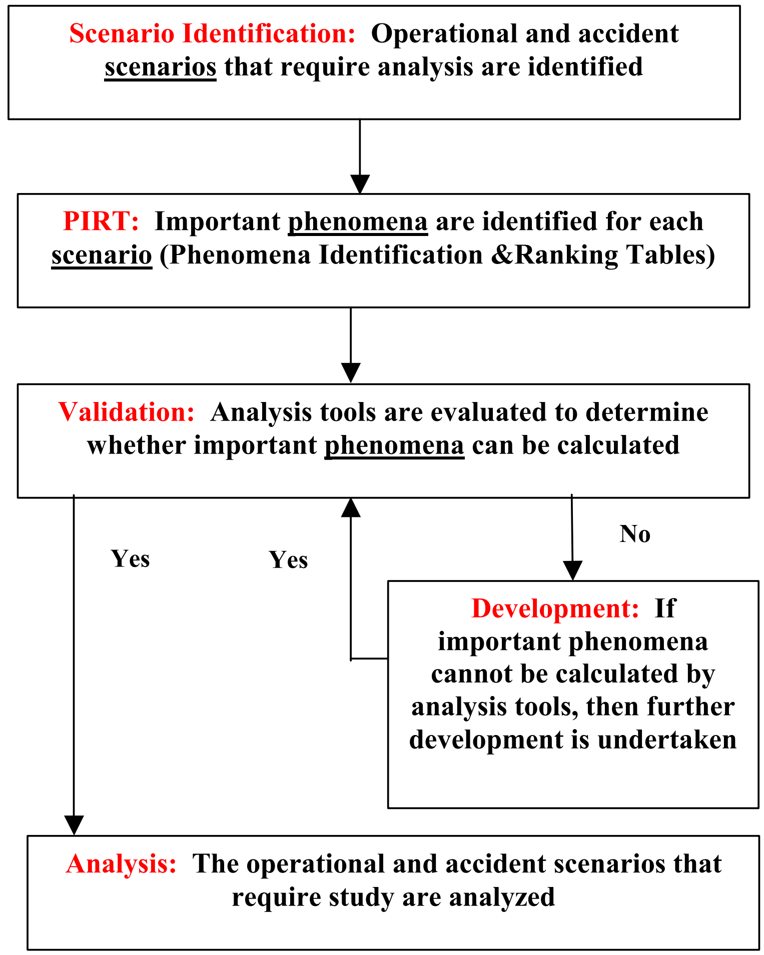


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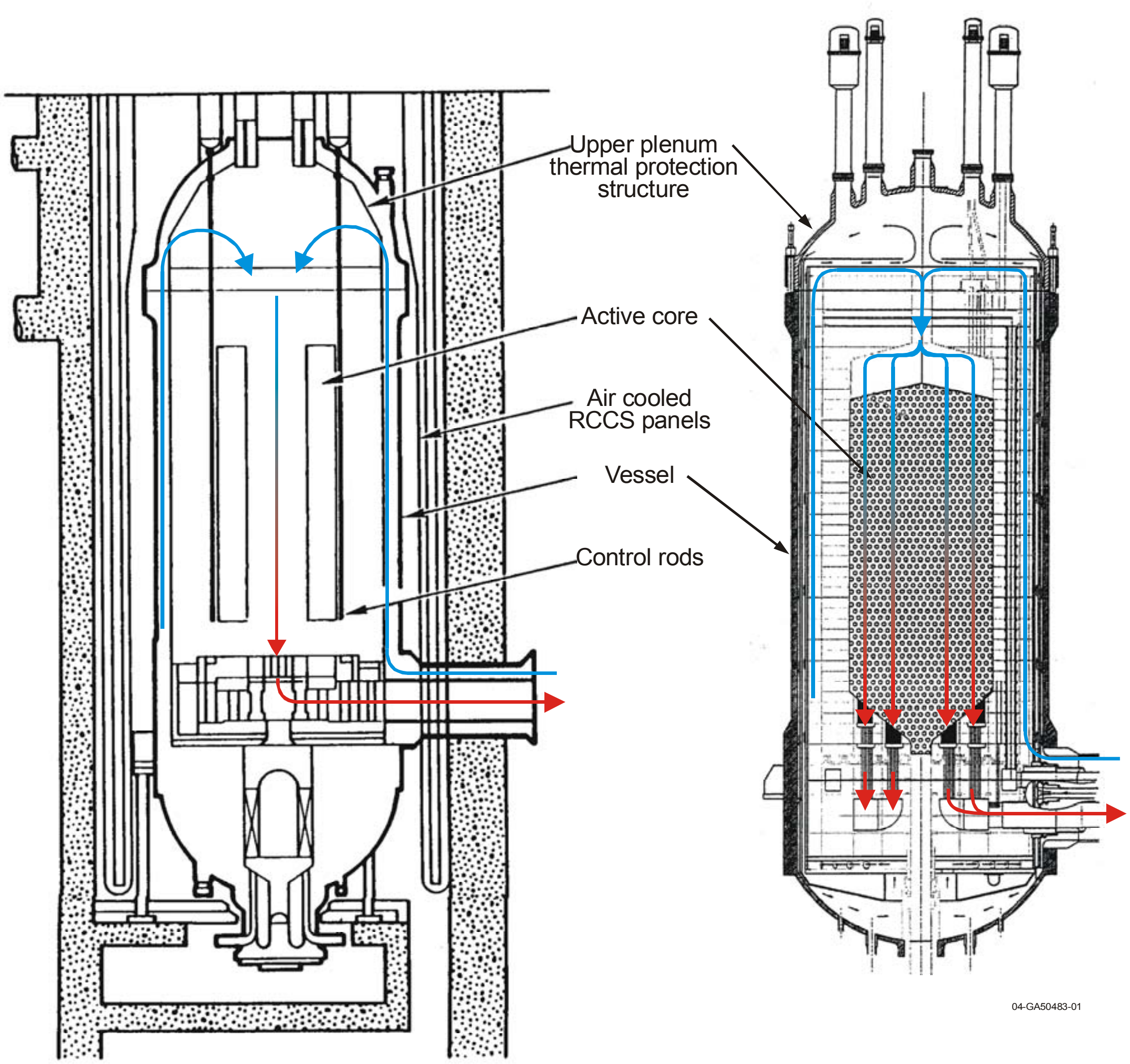
Figure 1. Research and development process.

2. NGNP DESCRIPTION

Typical prismatic and pebble bed advanced gas-cooled reactor configurations are shown in Figures 2a and 2b and typical operating specifications are given in Table 1 for 600-MWt rated operating power. MacDonald et al. (2003) briefly summarize the geometry and makeup of the two configurations.



a. Prismatic b. Pebble-bed

Figure 2. Typical very high temperature gas-cooled advanced reactor systems.

2.1 Configuration Description

The configurations of the two VHTR candidates are discussed briefly from the perspective of similarities and then differences. Where the two candidates have similar characteristics often the same analysis tools and the same R&D needs may be applied, e.g., computational fluid dynamics software. Where the candidates have marked differences unique software is sometimes required for each design, e.g., the analysis of the neutronic behavior in the pebble-bed design required the development of unique software (the PEBBED code—see Terry et al 2002) that is not applicable to the prismatic design.

Table 1. Typical specifications for reference VHTR designs.

Parameter	Direct Cycle Prismatic	Direct Cycle PBMR[c]	Comments
Power Output MWt)	600	600	
Plant Design Life (Years)	60	60	An extended plant lifetime requires operations that minimize the long-term stresses on the equipment.
Thermal Efficiencies (%)	48	45	High thermal efficiencies require innovative design and a multitude of optimization calculations.
Fuel enrichment (%)	15	8	To enable high fuel burnup to be achieved the fuel characteristics must be studied to ensure the optimal design is identified.
Fuel burnup (MWd/ton)	110,000	90,000	
Average power density (W/cc)	4	6.5	
System operational pressure (MPa)	7.1	7.1	These thermal-hydraulic boundary conditions form the basis for calculating "hot channel" behavior and the mixing characteristics in the vessel plena.
Inlet temperature (°C)	490	490	
Outlet temperature (°C)	1000	1000	
Flow rate (kg/s)	226	288	
Maximum fuel temperature (°C)	1276	1028	

Characteristics common to both configurations are:

- The working fluid is helium.
- The helium:

  a. Enters the vessel through either a circular cross-section pipe or a pipe annulus near the bottom of the vessel in a direction that is at right angles to the axis of the reactor vessel.

  b. Makes a 90-degree turn upward and is distributed into channels that lead upward to a plenum that is over the core itself.

  c. Is directed downward from the upper plenum into the core.

  d. Moves from the core into a plenum and is directed to a circular cross-section pipe (the hot duct) that is mounted at a right angle to the reactor vessel centerline. As the helium transits the core the gas temperature increases (by approximately 400 to 500 °C).

  e. Enters a second vessel and is directed to the to an intermediate heat exchanger or turbine inlet.

- The helium coolant flow distribution in the core is governed by the differential pressure between the upper and lower plena, the friction in the respective flow paths, and the local power generation.

[c] PBMR design tailored to NGNP needs.

- The moderator in both reactor configurations is graphite. Also the fuel in both consists of TRISO fuel-particles dispersed in a matrix even though the matrix for the prismatic design is cast in a fuel pin configuration while the matrix for the pebble-bed design is formed into a sphere.

- Both designs rely on forced flow, provided by blowers, of the helium coolant during operation.

- Both designs rely on passive cooling during any loss-of-power or loss-of-coolant scenario. The ultimate heat sink is the environment and all excess heat can be transported to the environment without natural circulation cooling inside the vessel via heat conduction and radiation to the vessel walls. From the vessel walls the heat is transported to the environment via a combination of radiation and natural circulation transport using some form of reactor cavity cooling system.

- Air is present in the containment (or confinement) such that if the reactor depressurizes due to a leak in a pipe, air will ultimately progress into the vessel by diffusion.

Fundamental differences between the two configurations stem largely from the differences between the fuels, such as:

- *Flow within the core:* The helium coolant, within the hexagonal blocks, follows well defined paths described by the coolant channels. However, an undefined quantity of bypass flow, ranging from ~10% to ~25% of the total coolant, moves between the blocks. The bypass flow varies according to the quality of the block construction, the shrinkage or swelling of the graphite as a function of irradiation and temperature, and the core stacking procedures. In contrast, the helium coolant moving through the pebble-bed core follows flow paths defined by the pebble-void fraction, which varies as a function of core radius, and the individual contact points described by the pebble column.

- *The pebble-bed core slowly moves downward while the prismatic core is stationary.* The cycle time through the core for an individual pebble is approximately 80 days. The transit distance is ~9.5 m.

- *The reactor kinetics and burnup characteristics are functions of the fuel and moderator geometry, the fuel enrichment, and the refueling characteristics of the respective designs.* Because the pebble-bed core is continuously being replenished as spent pebbles are removed from the system (each pebble is cycled through the core approximately 9 times), the pebble-bed core generally has a wider spectrum of depletion during operation than the prismatic reactor.

Due to the similarities between the prismatic and pebble-bed designs the same thermal-hydraulic tools can probably be used to perform the required analyses for both systems. However there will likely be validation requirements that are specific to each of these designs.

The major differences between the core configurations requires separate neutronic software for the prismatic and pebble-bed designs.

2.2 Operational Conditions

The neutronic and thermal-hydraulic behavior at rated operational conditions must be calculated to enable design studies to be conducted by INL and/or to perform audit calculations on designs submitted by potential NGNP commercial design teams. Such calculations are centered in two areas:

a. Calculation of the neutronic behavior of the proposed design include:

- Block loading studies for the prismatic design and pebble-loading for the pebble-bed design
- Block and/or pebble-bed k_∞ versus packing fraction
- Reactivity effects caused by the working fluid
- Model k-effective as function of temperature and core geometry
- Core k-effective versus core enrichment.
- Neutron flux, fluence, displacements-per-atom, and spectra
- Effect of water ingress on reactivity
- Fuel block depletion and pebble depletion
- Core depletion
- Temperature coefficients of reactivity
- Fuel rod power peaking and/or pebble power peaking.

b. Calculation of the thermal-hydraulic behavior of the system to determine:

- Helium gas exit temperature from hottest channel
- Variation in temperature between hottest and coldest jets into lower plenum
- Degree of mixing that occurs in the lower plenum and the translation of the temperature distribution to the IHX or turbine inlet
- Losses to the environment via the reactor containment cooling system, since this system is always operational
- Peak temperatures in the channels for the prismatic design and amongst the pebbles in the pebble-bed design. Peak temperatures in the structural members of both systems
- Evaluation of thermal stresses in fuel and system structural members.

2.3 Transient Conditions

The neutronic and thermal-hydraulic behavior during the most severe transient scenarios must be calculated to enable design studies to be conducted by INL and/or to perform audit calculations on designs submitted by potential NGNP commercial design teams. Such calculations are centered in two areas:

a. Calculation of the neutronic behavior of the proposed design include consideration of:

- Decay heat
- Local and global power imbalances resulting from inadvertent rod ejection (Morris et al. 2004)
- Water ingress.

b. Calculation of the thermal-hydraulics behavior of the proposed design include consideration of:

- Heat transfer to environment during conduction cooldown scenarios (both pressurized and depressurized)
- Peak temperatures in structural members
- Peak temperatures in fuel
- Mixing in the upper and lower plenums during PCC
- Natural convection and radiation heat transfer in reactor cavity cooling system.

3. R&D METHODOLOGY

This section describes the overall methodology used to define the R&D needed to produce the validated analytical tools required for the NGNP analysis. It consists of five steps: Scenario Identification, Phenomena Identification and Ranking, Analysis Tools, Validation, and Software Tool Selection. Each is described in the following subsections.

3.1 Scenario Identification

To show the NGNP meets all safety requirements, proven analysis capability must be available to model not only the operational conditions, but also the accident conditions. Also, various aspects of the core behavior must be modeled including:

(i) Operational characteristics of the TRISO fuel throughout the NGNP's life cycle, e.g., the fuel temperature profile, the migratory characteristics of the fuel kernel within the fuel micro-sphere, the shrinkage and swelling of the various pyrolytic carbon coatings, and the stress distributions in the coating layers.

(ii) Fuel power distribution as a function of exposure in both the fuel compacts or balls and in the micro-spheres.

(iii) Thermal-hydraulic conditions during both operating conditions and transient conditions, including the fuel temperature profiles and also the maximum temperatures of plant structural members such as the core barrel, core support plate, vessel wall, etc.

(iv) Mixing characteristics of the fluid inventory in the plena: the lower plenum during operating conditions since the hot exit gases are delivered to the IHX or turbine and both plena during a loss-of-forced flow scenario.

(v) Potential for air ingress and graphite oxidation subsequent to a loss-of-coolant accident (LOCA).

(vi) Fission product release and transport as a function of projected TRISO fuel failure rates.

For fiscal years 2004 and 2005 the highest priority R&D is aimed at properly calculating the thermal-hydraulic conditions in the hot channels and the mixing in the lower plenum during normal operation.

The full spectrum of possible accident scenarios of importance is not fully defined, since it is dependent on the presently undefined NGNP design. However, on the basis of the work done to license the Fort Saint Vrain reactor and the AVR reactor, it is known that the following scenarios, at least, must be analyzed, as indicated in the Fort Saint Vrain Final Safety Analysis Report (FSAR):

1. Anticipated operational occurrences:

    a. Main loop transient with forced core cooling
    b. Loss of main and shutdown cooling loops
    c. Accidental withdrawal of a group of control rods followed by reactor shutdown
    d. Small break LOCA (~1 in^2 area break).

2. Design basis accidents (assuming that only “safety-related” systems can be used for recovery):

   a. Loss of heat transport system and shutdown cooling system (similar to scenario 1b above)
   b. Loss of heat transport system without control rod trip
   c. Accidental withdrawal of a group of control rods followed by reactor shutdown
   d. Unintentional control rod withdrawal together with failure of heat transport systems and shutdown cooling system
   e. Earthquake-initiated trip of heat transport system
   f. LOCA event in conjunction with water ingress from failed shutdown cooling system
   g. Large break LOCA
   h. Small break LOCA.

On the basis of the experience of gas-cooled reactor designers and experimentalists (Ball 2003; Krüger et al. 1991), scenarios 2a and 2g [hereafter referred to as the Pressurized Conduction Cooldown (PCC) scenario and the Depressurized Conduction Cooldown (DCC) scenario respectively] are considered the most demanding and most likely to lead to maximum vessel wall and fuel temperatures. Hence, first-cut R&D specifications are based on calculation of the hot channel temperatures and mixing characteristics in the lower plenum during normal operation, and the PCC and the DCC scenarios from the accident envelope.

3.2 Phenomena Identification and Ranking Tables (PIRT)

The PIRT process entails carefully identifying the most demanding scenarios, followed by prioritizing the phenomena that are found in the most demanding scenarios. Key phenomena are those exerting the most influence on the path taken during the most demanding scenarios. Thus, as discussed in the previous paragraphs, the key phenomena for the PCC and DCC scenarios, or most “highly-ranked” phenomena, are those that exert the greatest influence on the peak core temperatures and peak vessel wall temperatures (ANS 2003). During normal operation other key phenomena such as stresses or irradiation induced dimensional changes may be important.

Because the specific NGNP design has yet to be selected, a detailed PIRT cannot be completed. However, during the interim, a “first-cut” or generic PIRT can be used instead as a guide for the initial R&D work and planning for both block-type and pebble-bed type gas-cooled reactors. The “first-cut” PIRT is based on (a) observations from seasoned gas-cooled reactor experts and (b) engineering judgment. Using this approach a PIRT generally applicable to gas-cooled systems has been documented in Vilim (2004). The results of the “first-cut” PIRT for normal operation, PCC, and DCC scenarios are given in Table 2. Terminology used in the table is described in the following paragraphs.

Mixing. Mixing refers to the degree to which coolant of differing temperatures entering a region mixes to produce a uniform temperature. In the plena (inlet and outlet), mixing is a three-dimensional phenomenon and a function of a number of variables. In the inlet plenum, where it is identified as important in the PCC scenario, mixing occurs during natural convection as helium moves upward through the hottest portion of the core while cooler helium moves downward through the bypass and the cooler regions of the core. In the outlet plenum, mixing occurs between the bottom of the core and the IHX or turbine inlet during normal operation. A preliminary calculation of the temperature variation in the lower plenum of the GT-MHR is shown in Figure 3 where gas temperature variations are shown to exceed over 100°C. Although the specification for temperature variation at the IHX or turbine inlet has not been set, it is thought that the helium temperature variation at the turbine inlet must be less than ±20°C. The allowable variation in temperature at the inlet of the IHX may be somewhat larger. Also, it has been seen that helium has a surprising resistance to thorough mixing [Ball 2004, based on experience of Kunitoni et al. (1986)] and that the temperature in the core outlet jet can vary over a considerable range, particularly since the bypass flow may vary between 10% and 25%. Therefore, it is likely that special design features will be required to ensure good mixing and minimal thermal streaking from the lower plenum to the turbine inlet.

Table 2. "First-Cut" PIRT for normal operation, PCC, and DCC scenarios.

Scenario	Inlet Plenum	Core	RCCS	Outlet Plenum
Normal operation		i. Neutronics behavior ii. Bypass flow iii. Hot channel characteristics		i. Mixing
DCC		i. Thermal radiation and conduction of heat across the core ii. Axial heat conduction and radiation iii. Natural circulation in the reactor pressure vessel iv. Air and water ingress. v. Potential fission product transport	i. Laminar-turbulent transition flow ii. Forced-natural mixed convection flow	
PCC	Mixing	i. Neutronics behavior ii. Bypass iii. Laminar-turbulent transition flow iv. Forced-natural mixed convection flow v. Hot channel characteristics at operational conditions	i. Laminar-turbulent transition flow ii. Forced-natural mixed convection flow	i. Mixing

Bypass. The bypass flow passes through the reflector regions in both pebble bed and block reactors and, in a block-type reactor, between the blocks. There may also be higher than normal flows in a pebble bed reactor near the reflector surfaces. Because the quantity of bypass flow is a direct function of the bypass area, which in turn is a function of the temperature distribution, fluence, and graphite properties, the influence of the bypass on the core temperature distribution may be significant.

Neutronics Behavior. The current NGNP design candidates have a somewhat harder thermal neutron spectrum than standard light-water reactors, a more complex fuel geometry, and a fuel cycle with two to three times the burnup. At the very high burnups expected for the NGNP, the higher isotopes of plutonium contribute a significant amount of fission energy. Yet the necessary cross section information, with the required accuracy, is unavailable from the current nuclear databases for ^{240}Pu, ^{241}Pu, and ^{242}Pu.

As an illustrative example of the current situation, Figure 4a shows a plot of the ENDF/B-VI data file values for the ^{240}Pu fission cross section (the black solid line), along with available published direct measurements over broad energy ranges in the same experiment shown by the colored vertical lines, with the length of the line as an indicator of the reported uncertainty of the data. Experimental data below ~10 eV are limited to single-point experiments that may or may not have been performed under the same conditions. Thus, in several energy ranges of interest, the ENDF values are heavily based on theoretical models with limited experimental data input, and can be highly uncertain. It should also be noted that even where data are available the reported uncertainties are high, for example, the capture cross-section for ^{240}Pu shown in Figure 4b. This capture cross section is of particular importance because neutron capture in ^{240}Pu leads to ^{241}Pu, which has a large (but also uncertain) fission cross section as well as a large capture cross section. Recent computational studies performed at INEEL show that for a reference

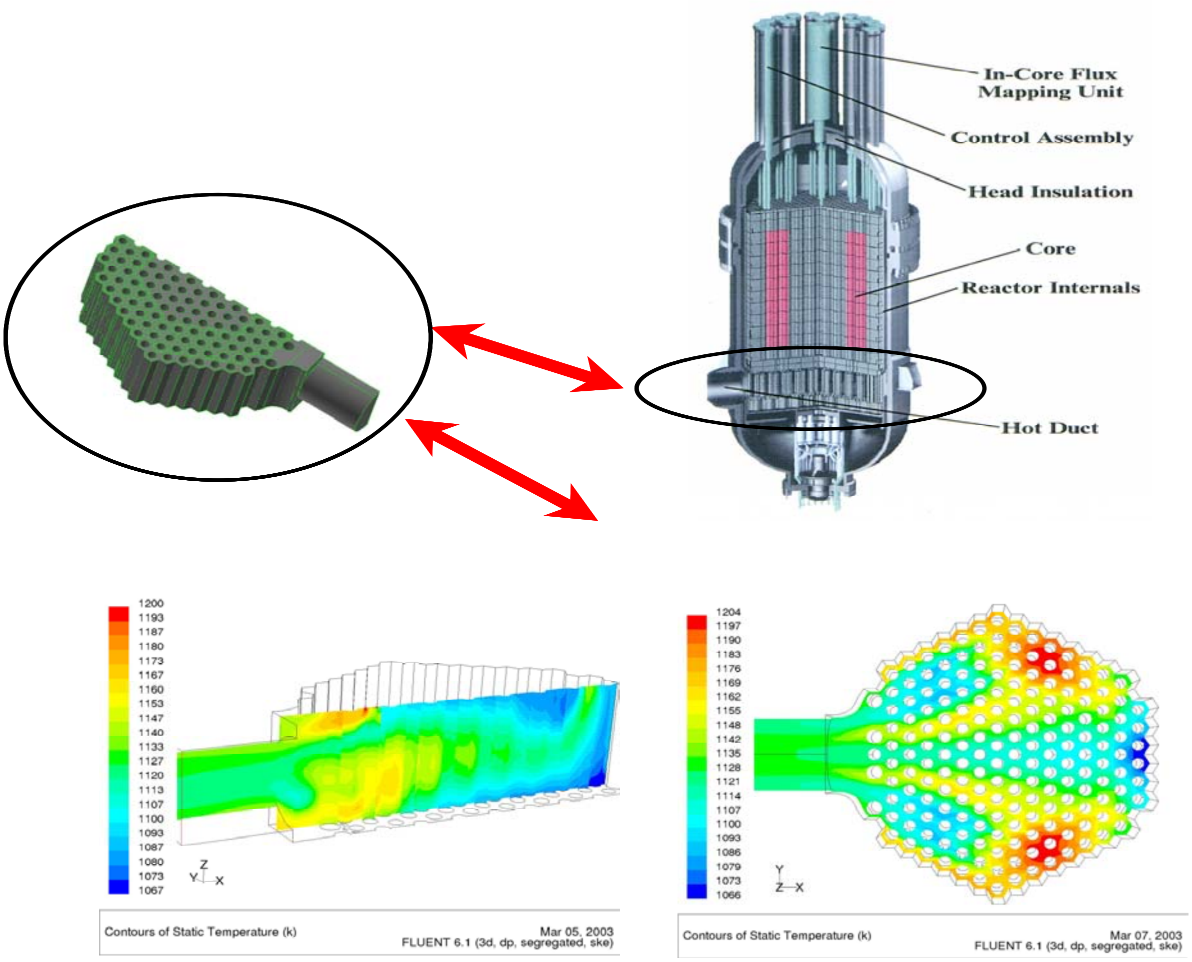
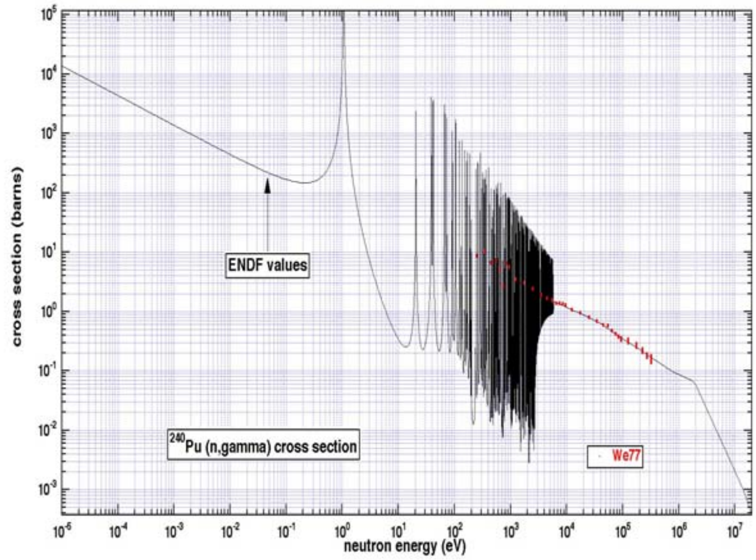


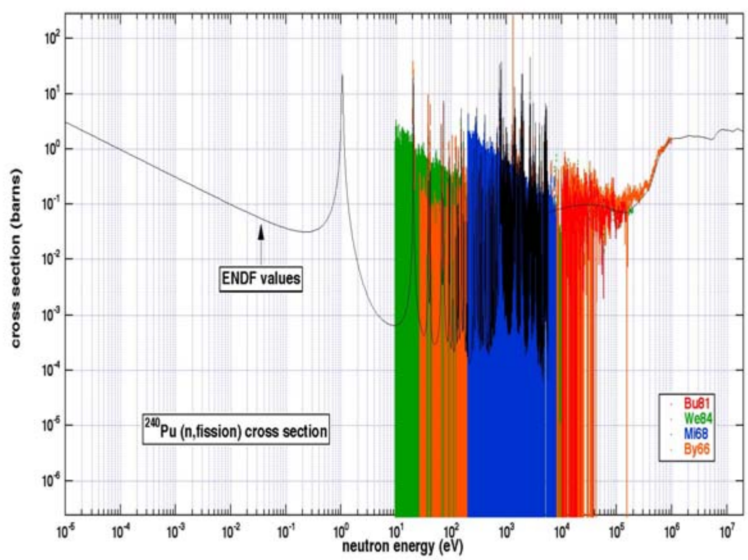
Figure 3. Computational fluid dynamics (CFD) calculation of mixing in lower plenum (courtesy of Fluent Corp).

prismatic NGNP fuel design, an uncertainty of as little as 10% in this cross section can lead to uncertainties in system reactivity of as much as 500 pcm absolute reactivity because of the propagated uncertainty in ^{241}Pu buildup. This is an indication of high sensitivity to this particular cross section. Furthermore, earlier integral-experiment-based code validation studies performed and published by INEEL (Sterbentz 2002; Sterbentz and Wemple 1996) for low-enriched fuel with thermal or slightly hyperthermal neutron spectra representative of typical NGNP designs show that computations of the inventories of the plutonium isotopes of interest here can vary by as much as 30% from corresponding measurements, at burnups of less than one-third of what is contemplated in a baseline NGNP scenario. Such discrepancies can propagate in a manner that can have major effects on the uncertainty of computed safety-related reactor parameters such as reactivity, Doppler feedback, etc.

In addition to improvements in the cross-section data to increase the accuracy of the neutronics calculations, improvements in cross-section processing methods are needed in the treatment of resonances in the thermal energy range in graphite-moderated reactors where upscattering is significant. The inability to account properly for this effect leads to substantial errors in the harder spectrum of a graphite-moderated reactor. Another aspect of improving cross sections is to account better for the heterogeneity on two scales in the NGNP. These two scales are the fine scale, from the fuel particles, and the coarse



(a) Fission



(b) Capture

Figure 4. ENDF/B-VI data file values, black solid line, and available experimental data sets for the ^{240}Pu fission and capture cross sections.

scale, from the pebbles or fuel compacts. The improvement in cross section generation will reflect enhanced resonance treatment through the use of an improved Dancoff factor.

Laminar-Turbulent Transition Flow and Forced-Natural Mixed Convection Flow. Figure 5 shows a likely layout for the NGNP with the reactor pressure vessel and the vessel containing the intermediate heat exchanger and primary coolant system circulator sited below grade. During the PCC scenario in the core region and during both the PCC and DCC scenarios in the reactor cavity cooling system (RCCS), there is the potential for having convective cooling in the transition region as shown in Figure 6, where an example of convection flow regimes along the heater (reactor core) and cooler (heat exchanger providing ultimate heat sink) at various pressures in a simplified Reynolds-Rayleigh number map (Williams et al. 2003) are plotted. Although Figure 6 was generated for a typical gas fast reactor core having hexagonal blocks with circular coolant holes, analogous behavior may occur in the NGNP in various locations and should be investigated. Because the convective cooling contribution is an important ingredient in describing the total heat transfer from the core and thus the ultimate peak core and vessel temperature, these heat transfer phenomena are potentially important.

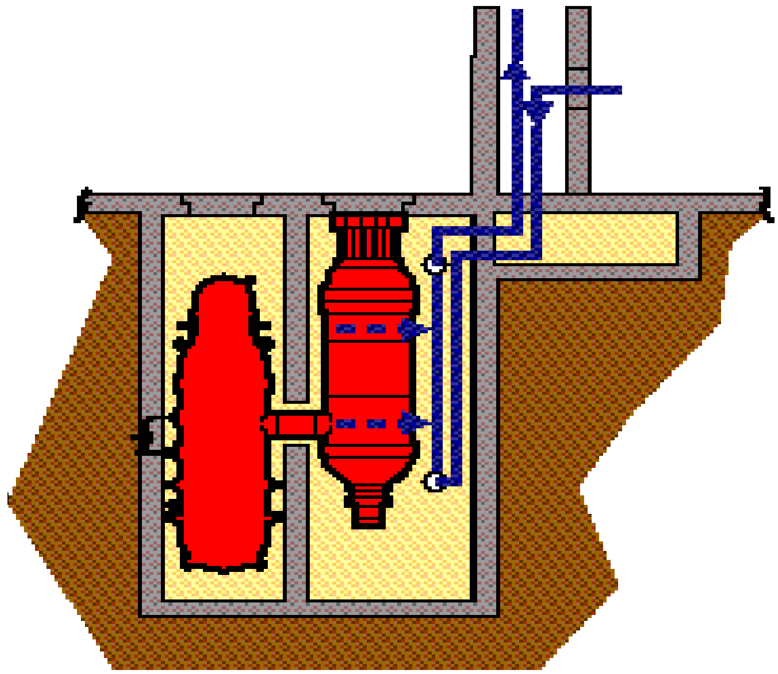


Figure 5. Reactor cavity cooling system configuration.

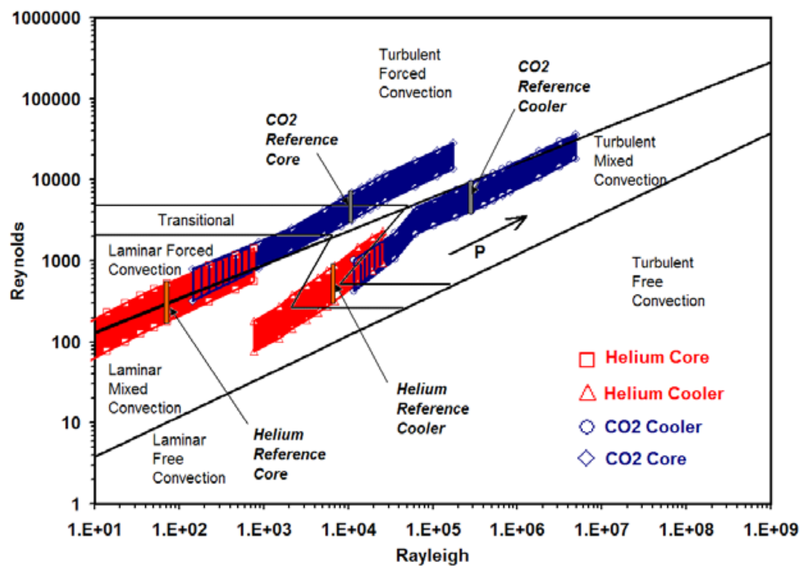


Figure 6. Convection flow regimes at various operating pressures for both helium and CO_2 (from Williams et al. 2003).

Core Hot Channel Characterization. The characteristics of the hottest cooling channels at operational conditions are considered a key calculational result since the hot channel temperature distribution defines the hottest initial condition for the fuel and surrounding materials. Hence preliminary computational fluid dynamics (CFD) studies have been initiated and validation data are sought.

Air & Water Ingress. For loss-of-coolant scenarios, such as the DCC, there is the potential for air and water ingress into the core in perhaps harmful quantities—depending on the scenario assumptions. Air will move into the core via diffusion and is present in the reactor cavity. Water is present in the air in the form of humidity but more importantly, may require consideration if the shutdown cooling system suffers a pipe break.

Fission Product Transport. Fission product transport must be calculated for cases where some fraction of the TRISO fuel particles fail prior to or in conjunction with the DCC scenario and because certain fission products such as silver and palladium may diffuse through the TRISO coatings. Dust, particularly for the pebble-bed reactor, that may contain fission products that must be tracked and accounted for using state-of-the-art calculational tools.

3.3 Analysis Tools and Data

The analysis requirements (items i through vi in Section 3.1) can only be achieved by using a spectrum of software tools and associated data libraries. For some calculational needs there are sometimes more than one software tool that may be used to achieve the calculational objective, each tool having a unique strength. To clearly illustrate the calculational process that satisfies the analysis requirements identified in Section 2 above, the process has been broken into the eight steps that are identified in Figure 7. Each of the eight steps are summarized in paragraphs a through h below; each paragraph item letter corresponds to a box on the flow chart shown in Figure 7. Figure 8 identifies the software associated with each of the steps in Figure 7.

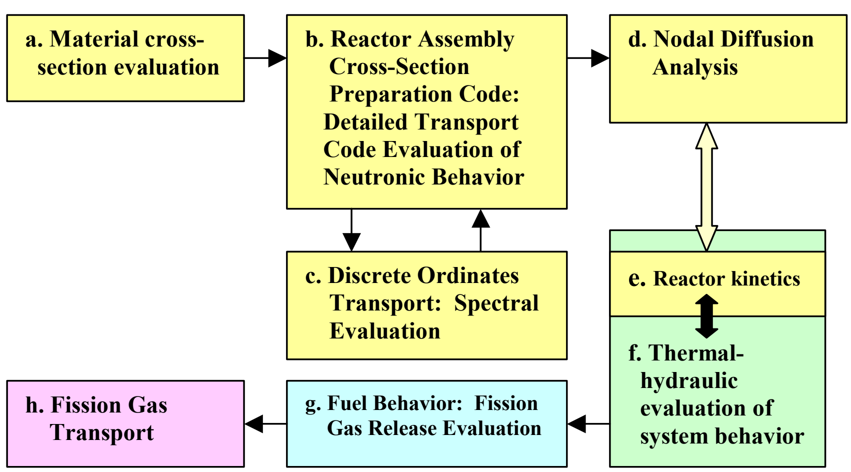


Figure 7. Complete calculation process.

a. Basic Nuclear Cross-Section Data Measurement And Processing. Nuclear interaction cross sections are among the most basic fundamental engineering data required for design, licensing, and operation of nuclear systems. The NGNP, in any of the currently envisioned configurations, will feature a neutron spectrum that is somewhat different from that in current light-water reactors, a fuel form that is more complex, and a burnup that is two to three times that of light water reactors. Studies noted previously, which will be extended as part of this R&D plan to provide additional detail, show that there is a near-term need for improved cross section measurements in certain neutron energy ranges for some isotopes to support the extensive computational modeling that will be required for the NGNP design regardless of the specific basic reactor configuration that is ultimately selected. The isotopes ^{240}Pu, ^{241}Pu, and ^{242}Pu are particularly important at high burnup as noted earlier.

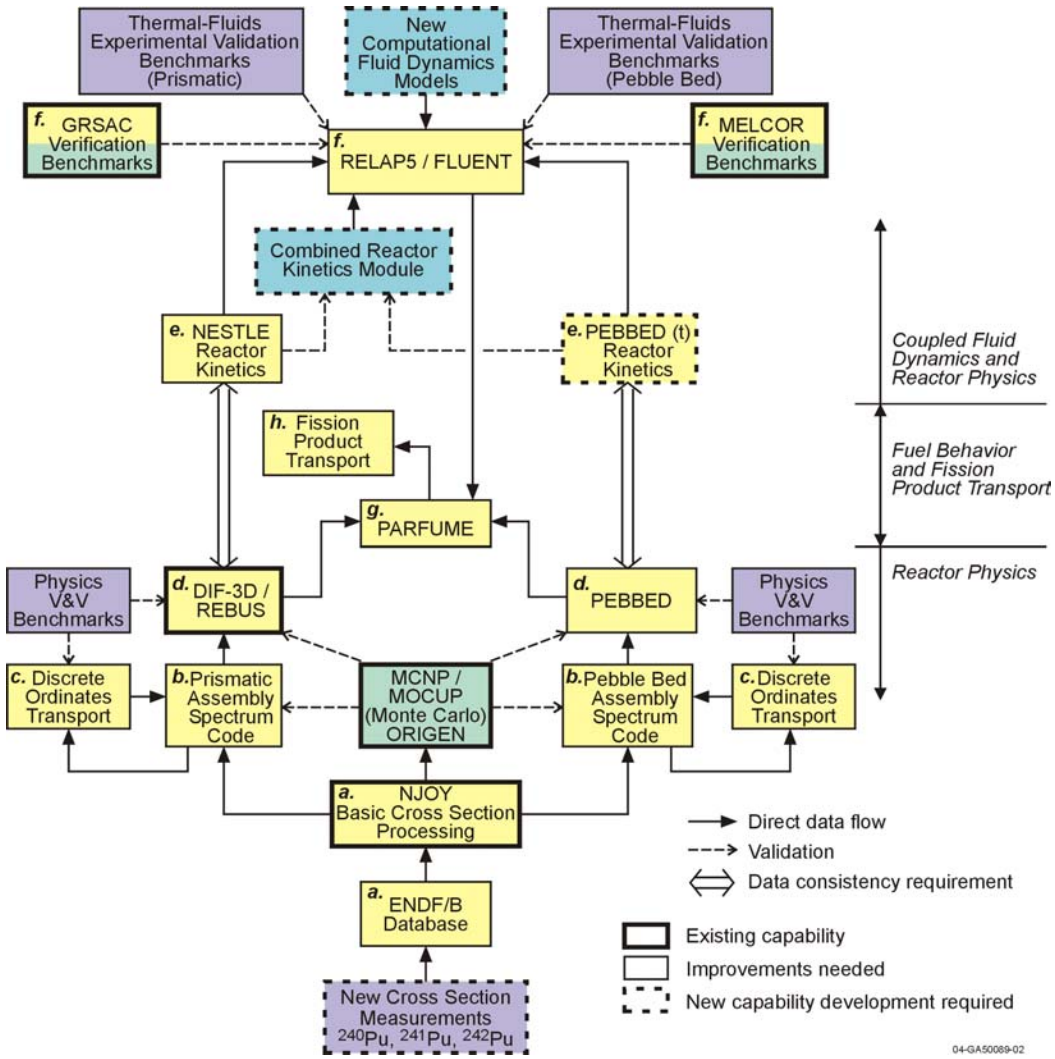


Figure 8. Application of process to block – type & pebble-bed candidate designs for NGNP—with application software.

b. Reactor Assembly Cross-Section Preparation. In order to use the ENDF cross-section data for a specific reactor application, the ENDF data, as processed into a general format by NJOY (MacFarlane and Muir 1994) or a similar tool, must be further processed into a case-specific form using local cell and assembly modeling codes as shown in Figure 8. The basic physical data are weighted with characteristic energy and spatial flux profiles generated from unit cell or supercell models. This step is performed using software that approximates the neutron transport equation using P_N or B_N transport codes for the energy flux calculation and a one- or two-dimensional transport code for the spatial flux. [In the advanced lattice codes, spatial resolution is typically done using integral transport methods (collision probability or method of characteristics approaches.)] Software that will be initially evaluated for this function includes

COMBINE (Grimesey et al 1991), BONAMI/NITAWL, MICROX-2 (Mathews 1997), WIMS-8 (AEA Technology), HELIOS (Stamm'ler et al 1996), and DRAGON (Marleau et al 1998), and an appropriate suite of codes will be implemented and validated according to accepted standards. Some geometric aspects of this process are somewhat different for the prismatic concept than they are for the pebble bed concept, so two computational paths are shown in Figure 8.

c. Discrete Ordinates Transport. To provide additional assurance that the computational results obtained using nodal diffusion theory codes are accurate, higher order, discrete ordinates transport should be employed to perform selective benchmark checks. Representative software that might serve this function is ATTILA (Wareing et al 1996), TWODANT (Alcouffe et al 1990), THREEDANT, or DORT/TORT (Rhoades et al 1992). These discrete ordinates packages are also used as part of the assembly cross-section preparation process (see Section b).

d. Nodal Diffusion Theory. Nodal diffusion-theory codes, such as DIF3D (Derstine 1984; Lawrence 1983; Palmiotti et al 1995) and an INEEL-developed code, PEBBED (Terry et al 2002), which is designed specifically for pebble-bed reactor simulation, will be the centerpiece production codes to perform NGNP reactor core analysis. Steady-state eigenvalues, energy and spatial flux profiles, reaction rates, reactivity changes (burnup and control rod movement), etc. will be calculated with the nodal diffusion-theory codes. Multi-group cross-section data generated in the reactor assembly cross-section preparation step (Step b above) will be provided to the nodal diffusion code. The DIF3D code also contains a nodal transport option (VARIANT) based on the variational transport approach. To consider the power behavior as a function of fuel depletion, additional capabilities are required. This function is usually performed by the REBUS code in conjunction with DIF3D, whereas it is internal to the PEBBED code for the PBR case. All of these software packages will be verified against alternate computational models, especially models based on the well known MCNP (Briesmeister 2000) stochastic simulation (Monte Carlo) code as shown in the center of Figure 8, and various discrete ordinates approaches as discussed below. In addition, all of the reactor physics models will be validated against various suitable experimental benchmarks. A preliminary assessment of appropriate validation benchmarks pertinent to the current NGNP reactor concepts is in fact already under way at INEEL and ANL under the Generation-IV program.

e. Reactor Kinetics. Output from the nodal diffusion codes will provide not only the steady state operational physics parameters for each operational analysis conducted but it will also be used as the initial condition for reactor kinetics calculations required as part of the overall system analyses performed in Step f below. Spatial changes in flux and power level as functions of time during postulated transients, predicted by the kinetics module, will provide the energy source term required for the overall thermal-hydraulic systems code computations at each time step during each transient. This process permits full coupling of thermal and neutronics computations, consistent with modern practice for nuclear systems analysis. The NESTLE (Turinsky et al 1994) code, a subroutine in the RELAP5 systems analysis thermal-hydraulics code, will serve this purpose for the prismatic reactor concept, and a time-dependent implementation of the PEBBED code will be used in the case of the pebble-bed concept.

f. Thermal-Hydraulics. The fluid behavior, and interactions with the neutronics, are calculated using a systems analysis code, or perhaps a coupled systems analysis/computational fluid dynamics (CFD) code. Examples of a systems analysis code and a CFD code are RELAP5 (RELAP5 2003) and Fluent (Fluent 2003). In such a coupling, systems analysis software are used to perform calculations of the overall system behavior considering the interactions between all the parts, e.g., the core, the plena, the hot exit duct, the turbine and the remainder of the balance of plant. CFD codes, such as Fluent, are used to calculate the detailed three-dimensional fluid behavior in a region of the reactor—such as the plena.

g. Fuel Behavior: The performance of fuel particles under irradiation and the determination of whether fuel failure occurs with the subsequent release of fission products is calculated to determine whether migration of fission products throughout the system must be considered. The software designed to perform this function is called PARFUME (Miller et al 2004). In addition to the physical description of the fuel, an operation history generated by physics and thermal analysis codes (consisting of fuel temperature, burnup and fast neutron fluence) are used as input to PARFUME. The code models the mechanical and physico-chemical behavior of the fuel and calculates the fraction of fuel particle failure. Several potential failure mechanisms are analyzed including cracking of structural particle layers, debonding of the inner pyrolytic carbon layer from the SiC layer, buildup of internal fission gas pressure, kernel migration (amoeba effect) to the SiC layer, and thinning of the SiC layer due to fission product interactions. PARFUME also calculates the fraction of selected fission product gases released from failed particles and from fission of uranium contamination in the matrix material surrounding the fuel particles. Calculation of release for selected metallic fission products is currently under development.

h. Fission Product Tracking. If a loss-of-coolant accident has occurred, such that the fission gas may migrate or be impelled into the confinement/containment building with perhaps subsequent release to the environment, then the final calculational step is the prediction of the fission gas movement into the environment and its environmental distribution.

The process described in items a through h is shown in the flow chart of Figure 7. The complete calculation process illustrated in Figure 7 is only exercised in its entirety for a few scenarios. Most scenarios would require the use of only a fraction of the calculations represented in Stages a through h. For example, scenarios that do not include a loss of coolant, i.e., a pipe break, usually would not require calculation of fission gas transport (Stage h). In addition, if the neutronics has been thoroughly calculated for the reactor system operating condition (Stages a through d), then a multitude of reactor system calculations can be performed using the evaluated reactor power state at time zero, and hence the Stage a through d calculations may only need to be performed once for a desired operating condition. Thereafter, for such scenarios that assume reactor scram (requiring no reactor kinetics: Stage e), a multitude of calculations can be performed using only the software tools developed for Stages f and g.

Some of the software tools that are planned for use in the calculation of the NGNP system will require both further development and validation. To date it is not certain which set of tools will be the ultimate focus of the NGNP process since the software tools are, to a degree, a function of the chosen reactor system, i.e., a block-type reactor or a pebble-bed reactor. Because the geometries of these two design candidates are different and also because the pebble-bed reactor system is dynamic (the pebbles are continuously being cycled and replaced depending on the exposure of individual pebbles), different software tools are used to analyze the behavior of the two fundamental designs as shown in Figure 8. For example, the nodal diffusion analysis (Stage d) software for the block-type reactor is DIF-3D while for the pebble-bed reactor it is PEBBED.

The various software associated with Stages a through h is given in Figure 8 for the block-type and pebble-bed reactor systems. Note that both the stages and the software are shown in three overall groups in Figure 8: (i) reactor physics, (ii) coupled fluid dynamics and reactor physics, and (iii) fuel behavior and fission product transport. The yellow-colored boxes represent the software applicable to Stages a through h as described above. Software that can be used to validate the behavior of other software, for limited applications, is indicated by a green color. For example, the MCNP software will be used to validate the behavior of the assembly spectrum codes (Item b) and the nodal diffusion codes (Stage d). Similarly, software such as GRSAC (Ball and Nypaver 1999) will serve to perform validation calculations for RELAP5 while also serving to perform selected systems behavior analyses (hence the GRSAC box is colored both yellow and green). Some of the software requires additional data and benchmark calculations. These functions are indicated by the lavender-colored boxes. Finally, the teal-colored boxes indicate the need for additional fundamental software development.

3.4 Validation

Whether or not software is adequate for performing best-estimate NGNP analyses is determined using both "top-down" and "bottom-up" evaluations as summarized in Figure 9 and described in the following sections.

"Bottom-Up" Code Adequacy: Bottom-up evaluation of code adequacy consists of four parts: examination of the pedigree, applicability, fidelity, and scalability of the code under consideration.

The pedigree of a systems code consists of its history, its development procedures, and the basis for each correlation that is used in the code. The correlations used in the code must be documented, e.g., in textbooks, laboratory reports, papers, etc. The uncertainty data used to bound the correlation(s) must be included in the documentation, e.g., instrumentation uncertainty, data system uncertainties, etc. The basis for the uncertainties should be traceable and reproducible. The assumptions and limitations of the models must be known and documented.

The applicability of a systems code depends on the range of use of each of its correlations. Those correlations must be documented and referenced. Finally, the range of applicability claimed in the code manual should be consistent with the pedigree—or if a greater range is claimed then the justification for the increase in range must be reported.

The fidelity of a systems code means the degree to which the code's predictions agree with physical reality. High fidelity requires that the correlations used in the code are not altered in an *ad-hoc* manner from their documented formulation. A code is validated when it is shown that the code's predictions of key parameters agree within allowable tolerances with experimental data. The validation effort should be complete for all the key phenomena in the events of interest. Finally, benchmarking studies may either supplement the validation effort or make up the validation effort if appropriate standards are available, e.g., comparison of code calculation with a closed form solution.

"Bottom-up" scaling stems from the need:

- To build experimental facilities that model the desired full-scale system.
- To closely match the expected behavior of the most important transient phenomena in the scenarios of interest.
- To demonstrate the applicability of data from a scaled facility to a full-scale system and to defend the use of data from a scaled facility in a code used to calculate the behavior of a full-scale system.
- To relate a calculation of a scaled facility to a calculation of a full-scale system.

Usually, scalability studies are performed to scale key parameters for a portion of the system behavior—not to correlate the global system behavior. Therefore, scalability analyses consist of four steps: (1) isolate the "first-order" phenomena, (2) characterize the "first-order" phenomena, (3) convert the defining equations into non-dimensional form, and (4) adjust the experimental facility conditions to give equivalent behavior with the full-scale system within the limitation of the facility (or nearly equivalent, i.e., based on non-dimensional numbers that follow from step 3).

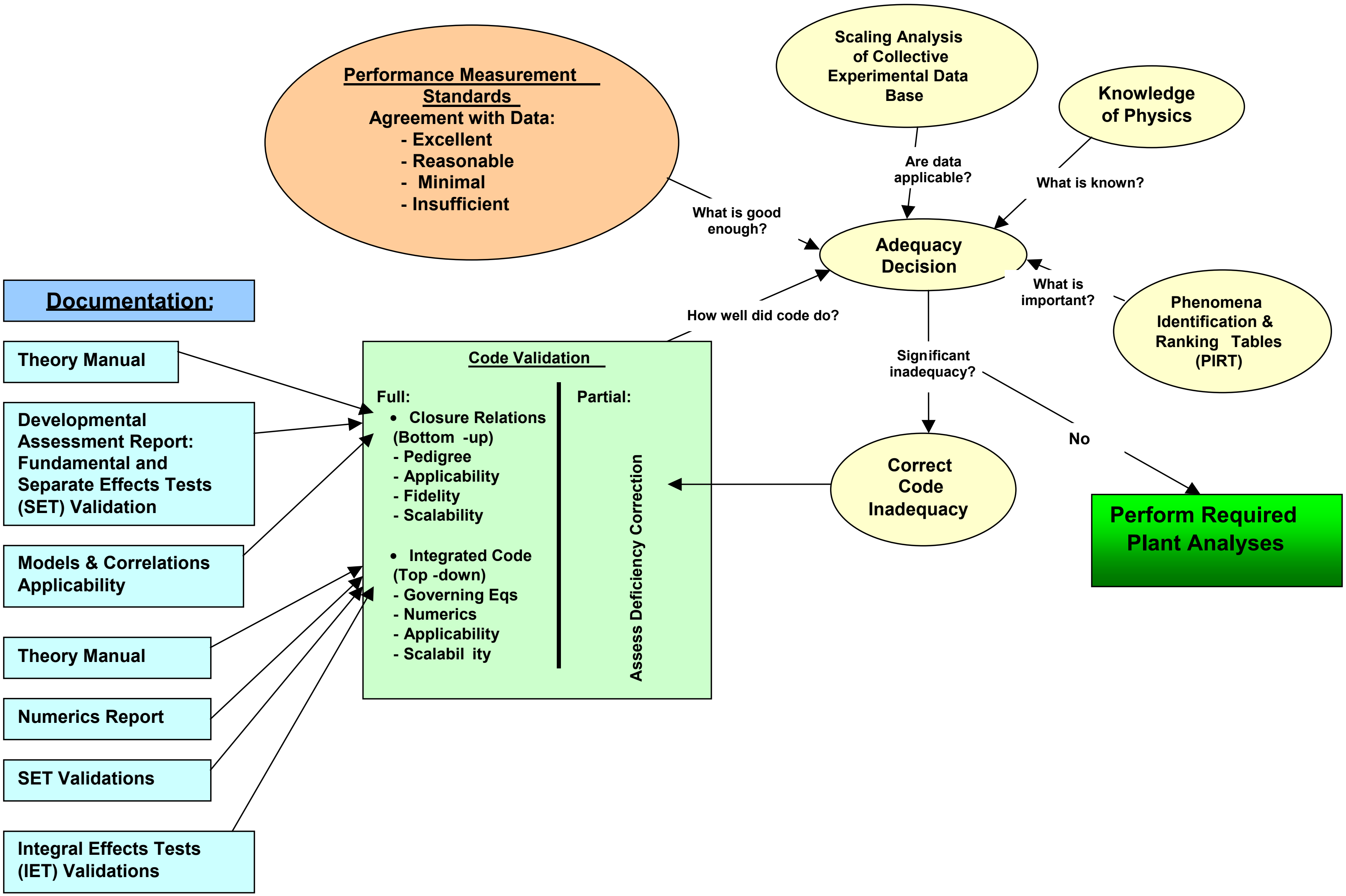


Figure 9. NGNP system design software: elements of adequacy evaluation and acceptance testing practices.

As implied in the above discussion, “bottom-up” code adequacy techniques focus principally on closure relationships.

Thus, the field equations used in the code must be correctly formulated and programmed. In addition, the field equations must be reviewed by the scientific community--and their agreement on the correct formulation and insertion of the governing equations in the code--must be obtained.

The “top-down” approach for ensuring code adequacy focuses on the capabilities and performance of the integrated code. The top-down approach consists of four parts: numerics, fidelity, applicability, and scalability.

Numerics: The numeric solution evaluation considers: (i) convergence, (ii) stability, and (iii) property conservation.[d] Again, agreement by scientific community on acceptable convergence, stability, and property conservation must be obtained.

Fidelity: The fidelity of the code is demonstrated by performing thorough code assessments based on applicable integral-effects and separate-effects data. The data are part of an agreed-upon code assessment matrix constructed based on the transients of importance and the key phenomena for each phase of the transients.

Applicability: The code must be shown capable of modeling the key phenomena in the system components and subsystems by conducting thorough validation studies. The key phenomena are identified in the Phenomena Identification and Ranking Table (PIRT).

The method to determine whether the code is capable of modeling key phenomena is done by comparing the calculation produced by the code to data that have known uncertainties. For example, “excellent” agreement between the code calculation and data is achieved if the calculated value is at all times within the data uncertainty band.

The degree of agreement between the code calculation and the data is generally divided into four categories—as given in Table 3. A more rigorous definition is given in Schultz, 1993. A code is

Table 3. Code adequacy identifiers.

Classifier	Description
Excellent	The calculation lies within or near the data uncertainty band at all times during phase of interest.
Reasonable	The calculation sometimes lies within the data uncertainty band and shows the same trends as the data. Code deficiencies are minor.
Minimal	Significant code deficiencies exist. Some major trends and phenomena are not predicted. Incorrect conclusions may be drawn based on the calculation without benefit of data.
Unacceptable	A comparison is unacceptable when a significant difference between the calculation and the data is present—and the difference is not understood. Such a difference could follow from errors in either the calculation or the portrayal of the data—or an inadequate code model of the phenomenon.

d. Property conservation issues arise when two calculations of the same property are performed by a systems code using two different algorithms or methods. This practice may follow in an effort to enhance the accuracy of the code result. Because the two methods are likely to calculate slightly different values of the same property, e.g., pressure, property conservation must be considered.

considered adequate in applicability when it shows either excellent or reasonable agreement with the highly-ranked phenomena (sometimes identified as the dominant phenomena) for a transient of interest. If the code gives minimal or unacceptable agreement, then additional work must be performed; the work may range from additional code development to additional analysis to understand the phenomena.

Scalability: Experimental scaling distortions are identified and isolated, e.g., inappropriate environmental heat losses that stem from the larger surface-to-volume ratios that are inherent to scaled facilities. Finally, an effort to isolate all code scaling distortions is performed through the code assessment calculations. Scaling distortions may arise from an inappropriate use of a correlation developed in a small-scale system when applied to a full-scaled system.

3.5 Software Tool Selection

When confronted with the need to calculate some of the phenomena that will be encountered in the NGNP scenarios, it is inevitable that analysts will be required to choose one software tool over another. This will be particularly true of systems analysis software (for example, GRSAC, MELCOR, and RELAP5—see Figure 8). To assist the analyst in formally choosing software, a methodology is given in Figure 10 where a flow chart summarizes key factors and questions such as:

a. The phenomena or scenario that requires analysis, as identified in the PIRT.

b. Has the software ever been used to analyze the phenomena or scenario? By answering this question the analyst may be introduced to references and other experts who have applied the software to similar phenomena or scenarios. Hence a body of useful information may be available.

c. Is the phenomena modeled properly? And does the model region of applicability correspond to the system phenomena or scenario envelope? These questions may be most easily answered by using the required manuals and documentation identified in Figure 9, e.g., models & correlations, theory manual, scaling relationships and applications, developmental assessment reports, validations, etc.

d. Have validation studies been completed for the phenomena or scenario? Were the validation results reasonable or excellent (as defined in Table 3)—or were the results minimal or unacceptable? If a body of validation results are not available, or if the validation results were not "reasonable" as a minimum, then the software should either not be used or it should be validated to ensure the calculated results are beneficial rather than misleading.

Only when acceptable answers are obtained for the questions listed above, can the software under consideration be used for the required analysis with confidence.

3.6 Quality Assurance Requirements: NGNP Methods Development R&D

- The systems design models to be used to analyze the behavior of the VHTR comprise the numerical models, correlations, algorithms, etc. that makeup the various software applications. These models also encompass the software input models that prescribe the design boundary conditions, e.g., operating conditions, geometry configuration, materials specifications, scenario description, etc. As discussed above, the systems design models will be used by the NGNP Project

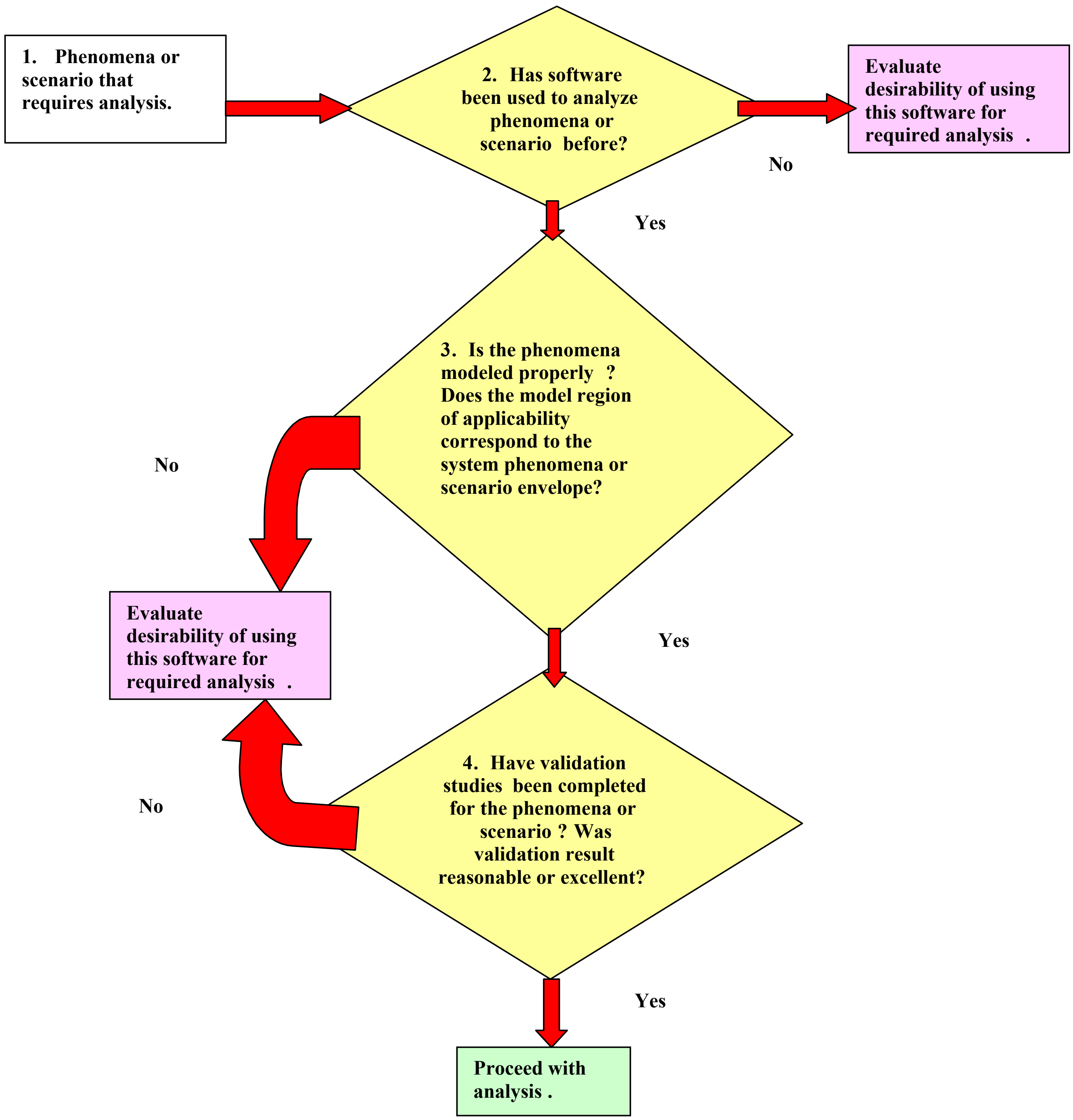


Figure 10. Flow chart to evaluate applicability of analysis software.

to assist in meeting most of the NGNP high-level functions, viz., to:

- Develop and demonstrate a commercial-scale prototype VHTR.
- Develop and demonstrate a high-efficiency power conversion system.
- Obtain licenses and permits to construct and operate the NGNP.

Because the NGNP is a nuclear facility, the U.S. national consensus standard ASME NQA-1-1997 (ASME 1997) applies—as noted in Chapter 4 of the NGNP F&R document (Ryskamp 2003) and the

Addendum to this document which deals specifically with systems design models (Schultz 2003). Consequently, the "Quality Assurance Requirements for Computer Software for Nuclear Facility Applications," as defined in Subpart 2.7 of NQA-1-1997 will be used as the basis for the NGNP systems design models requirements.

In addition to the NQA standards, since the analyses performed to evaluate the NGNP design performance and behavior using the systems design models may be used as a portion of the licensing submittal and requirements materials, the *Code of Federal Regulations, Title 10, Part 50* (10CFR50), Appendix B requirements also apply.

4. NUCLEAR DATA MEASUREMENTS, INTEGRAL EVALUATIONS, and SENSITIVITY STUDIES

High-accuracy differential nuclear data libraries as well as well-characterized and accurate integral benchmark information are required for all computational reactor physics tasks associated with NGNP design and subsequent operation. As noted previously, differential nuclear cross section data for all materials used in the reactor are required as input to the physics codes. Furthermore, integral benchmark experiment data for existing critical configurations that resemble the contemplated NGNP designs are required for physics code validation. Finally, mathematically rigorous sensitivity studies for representative NGNP core designs are required as an aid in prioritizing data needs and for guiding new experimental work in both regimes (differential and integral). The following three sections describe the near-term needs, planned activities, key milestones, and estimated funding requirements in these three areas.

4.1 Sensitivity and Uncertainty Studies

Although some relevant information is available from various previous studies, a mathematically rigorous theoretical evaluation of the uncertainties in computed core physics parameters that result from propagation of uncertainties in the underlying nuclear data used in the various modeling codes will be conducted early in the NGNP R&D effort. ANL has developed expertise in this area and will have the lead in this effort, which will serve as an aid in further quantifying the need for additional cross section measurements and/or evaluations for NGNP and as a guide in planning of future measurements and evaluations. This will be accomplished by performing formal sensitivity and uncertainty analysis based on perturbation theory in order to identify the nuclides that contribute to calculational uncertainties and to quantify the propagated uncertainties in the context of the currently anticipated likely NGNP core designs. The NGNP prismatic core design will be the basis for this initial study. Sensitivity coefficients will be calculated by generalized perturbation theory codes and folded with multigroup covariance data (where available) to derive propagated uncertainties in computed integral reactor parameters arising from the nuclear data. Potential integral parameters to be evaluated include reactivity, peak power, reaction rate ratios, nuclide inventory, safety coefficients, etc. The impact of cross-section data uncertainty on the accuracy of each parameter will be evaluated, along with the identification of nuclides, cross section types, and energy ranges that have greatest impacts on accuracy of integral parameters.

After the basic prismatic sensitivity study is completed in the first year, a broader campaign will be undertaken to install a capability at INEEL to enable a full partnership of INEEL with ANL in the conduct of additional sensitivity studies that will be required as the NGNP design evolves and new nuclear data measurements and evaluations are incorporated into the suite of computational tools for NGNP. Some neutronics code upgrades (for example development of an adjoint capability for the PEBBED code, as described elsewhere in this Plan) will also be necessary as part of this task, to allow treatment of both types of NGNP concepts. In addition to studies of nuclear data driven uncertainties, the capabilities to be developed in this program element will be needed for various other types of analyses. Examples include analysis of multivariate uncertainty propagation in connection with integral data evaluations described in the following section, studies of reactor kinetics parameters for various NGNP designs, etc.

Workscope for FY-05: Complete and document sensitivity study as described above for a representative prismatic core ($100K ANL)

Workscope for FY-06: Working with ANL, develop specifications for a sensitivity study appropriate to the Pebble Bed design and determine the computational needs required to complete this study. Sensitivities to various isotope uncertainties will likely be somewhat different in this case compared to the prismatic design, primarily because of the different asymptotic fuel loading pattern that will be attained. Install basic sensitivity study software capability at INEEL and initiate the PBMR sensitivity study in collaboration with ANL. ($100k INEEL; $100k ANL).

Workscope for FY-07: Complete the baseline PBMR sensitivity study in collaboration with ANL. Continue collaborative ANL/INL studies of uncertainties and sensitivities in NGNP system parameters as the system design evolves ($100 INEEL; $100k ANL).

Workscope for FY-08 and FY-09: Continue collaborative ANL/INL studies of uncertainties and sensitivities in NGNP system parameters as the system design evolves. ($100k INEEL; $100k ANL, each year).

Total funding needs: FY-05 through FY-09 = $900k.

4.2 Integral Nuclear Data Evaluations

Computer codes used in design and safety analyses of the NGNP must be shown *a priori* to be able to model NGNP configurations accurately. Therefore, these codes must be benchmarked against appropriate available experimental data. Various experimental data on the reactor physics of high-temperature reactors (HTRs) have been measured internationally since the early 1960s. During FY-04, under DOE Gen-IV crosscut funding, the INEEL and ANL studied all the known experimental and prototypical HTGRs and relevant critical facilities in order to assess their potential to be used as benchmarks. The facilities that have been assessed for the pebble-bed type NGNP are ASTRA, AVR, CESAR II, GROG, HTR-10, HTR-PROTEUS, KAHTER, SAR, and THTR. The facilities that have been assessed for the prismatic block type NGNP are DRAGON, Fort St. Vrain, Gulf General Atomic (GGA) criticals, HITREX-1, HTLTR, HTTR, MARIUS IV, the Peach Bottom Reactor, Peach Bottom criticals, SHE, U.K. NESTOR and HECTOR lattices, and VHTRC.

Design and safety analysis calculations for the NGNP will require calculation of k-effective, neutron flux distribution, and reaction rates and cross sections, along with quantities that can be derived from flux and cross sections such as depletion, power distribution, etc. To confirm that analysis codes can predict these quantities with sufficient accuracy, the codes must be benchmarked against experimental measurements made in the closest possible conditions to those expected in the NGNP. Conditions relevant to benchmarking NGNP codes include geometry, fuel type, and, for a pebble-bed-type experimental facility, whether it achieved an asymptotic state. Code-calculated quantities to be compared with experimental data include k-effective, flux distributions (where measured values are available), and spectral indices (key reaction rate ratios used to determine whether the neutron energy spectra are comparable). Finally, a key concern in selecting appropriate benchmarks is related to whether the required data are readily available from an experimental facility.

Tables 4 and 5 compare the facilities discussed above with respect to various qualities desired for use in benchmarking computer codes. One of the column headings has different meanings in the two tables. A pebble-bed reactor operating at constant power for a sufficiently long time (on the order of two or three years) will approach asymptotic distributions of neutron flux and compositions. In principle, except to replace radiation-damaged reflector components, the pebble-bed reactor never needs to be shut down, so these asymptotic distributions will be approached more and more closely as time goes on. Prismatic-type reactors are batch-loaded, so the compositions change continuously with time. They do not approach asymptotic distributions as pebble-bed reactors do, and operation is interrupted at intervals of roughly 18 to 24 months for fuel removal, shuffling, and replacement. However, after several operating cycles, the distribution of compositions at cycle startup approaches an asymptotic configuration.

Table 4. Comparison of facilities relevant to codes for modeling pebble-bed-type core.

Facility	Geometry	Size	Fuel type	Asymptotic state or zero-power startup	Availability of data	Priority
ASTRA	Annular, but not azimuthally symmetric	Small	As desired	Zero-power startup	Existing facility – data can be obtained	High
AVR	Cylindrical	Short; radial extent appropriate	Various; some low-enrichment TRISO	Both	Uncertain	High
CESAR II	Hexagonal	Small	Low-enriched UO_2	Zero-power startup	Neutronics data exist	Medium
GROG	Cylindrical or annular	Short; radial extent appropriate	As desired, but very low packing fraction	Zero-power startup	Existing facility – data can be obtained	Medium
HTR-10	Cylindrical	Small	Low-enriched TRISO	Both	Existing facility- data can be obtained	Highest
HTR-PROTEUS	Cylindrical	Small	LEU pebble-bed fuel	Zero-power	PSI and IAEA would need to be contacted	High
KAHTER	Cylindrical	Small	Uncertain	Zero-power startup	Uncertain	High
SAR	Cylindrical	Small	Probably low-enrichment TRISO	Zero-power startup	Limited data were obtained for this special-purpose test	Low
THTR	Cylindrical	Large	Thorium-uranium	Most data for zero power; reactor presumably achieved steady state	More data available for zero-power startup than operating conditions	Medium

The column heading “Asymptotic state or zero-power startup” refers to the true time-independent asymptotic configuration for pebble-bed reactors, but to the cycle-independent startup configuration for prismatic-type reactors.

Trends were observed in the experiments that were performed in the various facilities investigated. It was found that most of the experiments for block-type cores were performed in the United States, while those on pebble-bed cores were done predominantly in Europe. Most of the early U.S. experiments used highly enriched uranium. This was not typically the case for the European experiments. Additionally, experiments are currently being performed for both pebble-bed and block type cores in Asia (Japan and China) as well as in Russia. Under this NGNP program element, we will have the opportunity influence the direction of these experiments in a way that enhances the specific benefit to the NGNP effort.

Table 5. Comparison of facilities relevant to codes for modeling prismatic block type core.

Facility	Geometry	Size	Fuel type	Asymptotic state or zero-power startup	Availability of data	Priority
DRAGON	Hexagonal	Small	HEU/Th	Both	Data must be retrieved from U.K./OECD	Low
Fort St. Vrain	Cylindrical	Large	HEU/Th	Both	Data is GA proprietary	Medium/ High
GGA HTGR criticals	Cylindrical	Small	HEU	Zero	Data is GA proprietary	Medium/ High
HITREX-1	Hexagonal	Small	LEU fuel	Zero	U.K. nuclear data	Medium/ High
HTLTR	Block	Small	Pu-Th fuel	Zero	PNNL data	Low
HTTR	Cylindrical/ Annular	Small	LEU fuel	Both	Existing facility- data can be obtained	High
MARIUS-IV	Unknown	Small	HEU-Th	Zero	Unknown	Low
Peach Bottom HTGR	Cylindrical	Small	HEU/Th	Both	Data is GA proprietary	Low
Peach Bottom Criticals	Cylindrical	Small	LEU/Th	Zero	Data is GA proprietary	Low
SHE	Hexagonal	Small	LEU fuel	Zero	JAERI data	Medium/ High
NESTOR/ HECTOR	Square and cylindrical	Small	LEU fuel	Zero and elevated temperatures	U. K. nuclear data	Medium/ High
VHTRC	Hexagonal	Small	LEU fuel	Zero	JAERI data	High

The HTGR cores have evolved to improve system economy and safety. The NGNP core concept, one of the most advanced, has many different technical aspects compared to those of the early HTGRs. The evolution of the core limits the applicability and usefulness of the existing experimental data to NGNP core designs. Additionally, in the case of the data produced on national or commercial bases, the availability of those data might be quite limited.

This preliminary assessment revealed that five experimental data and facilities have the highest priority for pebble-bed type cores. These are the HTR-10, AVR, HTR-PROTEUS, ASTRA and KAHTR. In terms of data applicability and availability, the HTTR and VHTRC data were rated highly as being directly pertinent to the evaluation of the pedigree of data and tools used for the design and analysis of block-type NGNP cores.

Given the assessment of available data in FY-04, as described above, the next steps under this R&D plan will involve detailed evaluation and documentation of the selected high-priority benchmarks to provide benchmark specifications that are accepted by the community and by regulators for validation of physics modeling codes. The work will be conducted under the auspices of the International Reactor Physics Evaluation Project (IRPhEP) an international effort that was endorsed by the Organization of Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) in June of 2003. While coordination and administration of the IRPhEP takes place at an international level, each participating country is responsible for the administration, technical direction and priorities of IRPhEP-sanctioned evaluation activities conducted within their respective countries. Thus, the INEEL (with ANL participation) will contribute NGNP-specific benchmarks evaluated under this R&D Plan. Data contributed to the IRPhEP will be published in an OECD Handbook that will be made available to all participating countries. Because of the rigorous quality standards involved in the evaluation process, published IRPhEP benchmarks will have the highest reasonably achievable level of international credibility and acceptance.

Protocols for the IRPhEP are patterned after those of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) for evaluation and preservation of integral data suitable for validation of physics codes data used for ex-core nuclear criticality safety assurance. The IRPhEP is closely coordinated with the ICSBEP in order to avoid duplication of effort (both projects are managed through the INEEL and the OECD-NEA NSC—with ANL participation). Some Benchmark data are applicable to both nuclear criticality safety and reactor physics technology. Some have already been evaluated and published by the ICSBEP; however, ICSBEP efforts are focused primarily on non-reactor critical configurations and have, in general, only mentioned in passing other types of measurements relevant to reactor cores such as reactivity measurements, flux distributions, spectral indices, reaction rates, β_{eff}, etc. Experiments that are relevant to reactor physics applications that have already been evaluated and published by the ICSBEP will simply be extended by the IRPhEP to include evaluation and documentation of other reactor physics measurements that were made in conjunction with the assembly of a critical configuration. Measurements that have not been evaluated by the ICSBEP, such as the NGNP-relevant experiments discussed in this R&D Plan will be fully evaluated and documented in accordance with similar guidelines, requirements, and quality assurance measures as apply to the OECD-ICSBEP.

The INEEL provides leadership for the IRPhEP Technical Review Group that was organized during FY 2004 / FY 2005 as noted above, maintains the infrastructure of the IRPhEP, and is responsible for compiling and distributing annual publications. ANL will also participate in this activity. Based on experience with the ICSBEP, DOE will realize significant benefits. Through this effort the IRPhEP will be able to (1) consolidate and preserve the information base that already exists worldwide; (2) retrieve lost data; (3) identify areas where more data are needed; (4) draw upon the resources of the international reactor physics community to help fill those needs; (5) identify discrepancies between calculations and experiments due to deficiencies in cross section data, cross section processing codes and neutronics codes; (6) eliminate a large portion of the tedious and redundant research and processing of reactor physics experiment data; and (7) improve experimental planning, execution, and reporting.

The formal benchmark evaluation process is quite rigorous and includes the following basic steps performed for a given benchmark by the evaluating organization:

1. Verify the data, to the extent possible, by reviewing original and subsequently revised documentation, and by talking with the experimenters or individuals who are familiar with the experimenters or the facility.

2. Develop analytical models for the specific core configuration measured using standard computer codes and, in the case of this R&D plan specific to NGNP, using the codes specifically intended for NGNP analysis.

3. Perform appropriate computations and compare the results with the associated experimental data.

4. Compile the data and the methodologies (experimental and analytical) into a standardized format.

5. Evaluate the data and uncertainties associated with the data.

6. Formally document the work into a single source of verified reactor physics measurements data.

Each draft experiment evaluation then undergoes thorough internal review by the evaluator's organization. Reviewers verify the following:

- The accuracy of the descriptive information given in the evaluation by comparison with original documentation (published and unpublished)
- That the benchmark specification can be derived from the descriptive information given in the evaluation
- The completeness of the benchmark specification
- The results and conclusions, and adherence to format.

In addition, each experiment undergoes independent peer review by another IRPhEP Technical Review Group member at a different facility. Starting with the evaluator's submittal in the appropriate format, independent peer reviewers verify:

- That the benchmark specification can be derived from the descriptive information given in the evaluation
- The completeness of the benchmark specification
- The results and conclusions
- Adherence to format.

A third review by the assembled IRPhEP Technical Review Group then verifies that the benchmark specification and conclusions are adequately supported.

The NGNP integral evaluation activities conducted by INEEL under this Plan, with ANL participation, will be coordinated with the ongoing Generation-IV Design and Evaluation Methods Crosscut program to avoid duplication of effort and to maximize funding leverage. It is planned to perform a detailed evaluation suitable for submittal to peer review of one critical integral experiment during FY-05, prioritized according to the assessment exercise completed in FY-04, with the final selection consistent with overall plans developed in the October, 2004 meeting of the IRPhEP Technical Review Group in Paris. The first experiment to be evaluated will most likely be either the HTR-10 facility in China, the ASTRA facility in Russia, or the AVR facility in Germany in the case of the Pebble Bed concept, or possibly a high-priority prismatic concept, depending on availability of data in the near term and the commitments made to perform evaluations by other IRPhEP participants. In the following years INEEL will continue to evaluate and submit additional NGNP-relevant benchmarks at the rate of at least one per year.

Work scope:

- FY-05: $220K, based on matching of anticipated FY-05 Gen-4 Crosscut funding for related activities.

- FY-06 and beyond: Estimated at $460K per year (plus approved escalation) based on the assumption that NGNP-specific work of this type will be supported entirely by NGNP resources in the out years and that the Crosscut effort will be somewhat more general in nature (support of US IRPhEP participation, development of benchmarks for other Gen-4 concepts, etc.). This level of resources will cover necessary travel, INEEL labor, and will allow involvement of students in the evaluations.

- An additional $120k per year in FY-07 and beyond will also permit a parallel effort to develop recommendations for new benchmark experimental measurements as the NGNP design evolves (e.g. decision on pebble bed or prismatic design) and specific needs are clarified in the context of the ongoing detailed evaluations described here for existing data identified in the assessment document developed in FY-04.

- Total funding needs FY-05 to FY-09: $2,420k.

4.3 Differential Nuclear Data Measurements

Studies already conducted by INEEL and others as a part of the NGNP, Generation-IV, and Advanced Fuel Cycle (AFC) programs show that the transuranic nuclides, for which useful cross section data is extremely limited in many cases, will in fact dominate the neutronic behavior of some advanced nuclear energy systems of interest, especially at high burnup. Yet the necessary cross section information, with the required accuracy, is unavailable from the current nuclear databases for some key nuclides of interest. Integral experiment studies (e.g., Mercatali et al. 2004) confirm the sensitivity of computed parameters to uncertainties in the cross sections of many of these materials. In the case of the NGNP the current design is envisioned to feature a somewhat harder thermal neutron spectrum than is often the case for standard light-water reactors, a more complex fuel form, and a fuel cycle with two to three times the burnup. As a result, there is a need for improved cross section measurements in certain neutron energy ranges for some isotopes, in particular ^{240}Pu, ^{241}Pu, and ^{242}Pu.

Reviewing the previously summarized illustrative example of the current situation, Figure 4a shows a plot of the ENDF/B-VI data file values for the ^{240}Pu fission cross section (the black solid line), along with available published direct measurements over broad energy ranges in the same experiment (shown by the colored vertical lines), with the length of the line as an indicator of the reported uncertainty of the data. Experimental data below ~10 eV are limited to single-point experiments that may or may not have been done under the same conditions, as discussed later. Thus in several energy ranges of interest, the ENDF values are heavily based on theoretical models with limited experimental data input, and can be highly uncertain. It should also be noted that even where data are available the reported uncertainties are high. Figure 4b shows the capture cross section for ^{240}Pu. In this case the experimental data are even more limited and no uncertainties were reported. This capture cross section is of particular importance because neutron capture in ^{240}Pu leads to ^{241}Pu, which has a large (but also uncertain) fission cross section as well as a large capture cross section. Recent computational studies performed at INEEL show that for a reference prismatic NGNP fuel design, an uncertainty of as little as 10% in this cross section can lead to uncertainties in system reactivity of as much as 500 pcm absolute reactivity because of the propagated uncertainty in ^{241}Pu buildup. This is an indication of high sensitivity to this particular cross section. Furthermore, earlier integral experiment based code validation studies performed and published by INEEL (Sterbentz 2002; Sterbentz and Wemple 1996) for low-enriched fuel with thermal or slightly hyperthermal neutron specta representative of typical NGNP designs show that computations of the inventories of the plutonium isotopes of interest here (A=240-242) can vary by as much as 30% from corresponding measurements, at burnups of less than one-third of what is contemplated in a baseline NGNP scenario. Such discrepancies can propagate in a manner that can have major effects on the uncertainty of computed, safety-related, reactor parameters such as reactivity, doppler feedback, etc.

A comprehensive standard database, CINDA (Computer Index of Neutron Data), maintained by the National Nuclear Data Program at Brookhaven was used as the source for the experimental data files and references on ^{240}Pu shown in Figure 4. On searching CINDA, 1450 references and data files were found. Not all of the 1450 references are reporting experimental results as these references include papers on evaluations, theoretical calculations and models, and papers without data values. Of these, only one direct measurement of the neutron capture cross section over an extended energy range under self-consistent conditions was found. All other capture cross section information was extracted from ratio measurements relative to other nuclides, was based on calculational extractions from total neutron induced reactions on a ^{240}Pu sample, or was composed of single point measurements at one energy or averaged over an energy range to yield a single value. The vast majority of the single point values were at "thermal" energies or were integral values.

The summary point is that the roughly 50,000 points in the ENDF data file for the ^{240}Pu capture cross section are the result of one or more nuclear model calculations with very limited experimental data as input. There are 18 experimental data files (i.e., there are 18 experimental references in the 1450 CINDA references that represent any experimental measurement) with only one file containing a direct measurement with experimental results over an energy range. The 17 other experimental data files used in compiling the ENDF file are total cross section measurements, ratio measurements, or single point measurements. As another example, there are 810 references in the CINDA database for the ^{240}Pu fission cross section. Of these, 40 references have experimental data of some form that are used to construct the ENDF evaluated file containing 50546 data points. The four experimental data files that are plotted represent the only direct, multipoint measurements of the cross section out of the 40 references containing experimental cross section values. The other 36 references of experimental data sets are either ratio measurements, single point measurements, or average values over several broader energy ranges. The single point values are Maxwellian distributions about some central energy values, generally 0.025 eV. The 810 ^{240}Pu fission cross section references in CINDA also contain experimental data on other parameters (nu, yield, average kinetic energy) associated with fission as well as evaluations, theoretical papers, reports and other works that do not contain direct data.

It should also be noted that the situation for ^{242}Pu is similar to what was described in greater detail above for ^{240}Pu, as illustrated by see Figures 11 and 12. For the actinides other than ^{235}U and ^{239}Pu, this is the common situation, as the experimental effort has not been put into measurements for these actinide isotopes compared with the case for ^{235}U and ^{239}Pu. In the longer term there is thus also a need for new data for essentially all of the other (approximately 16) heavy actinides that will come into play with the even more advanced Generation-IV systems and fuel cycles under study. However, the emphasis in this discussion, specific to NGNP, is on the plutonium isotopes previously noted. It should also be noted that for reasons outlined below there is also appropriate justification to perform some initial measurements using ^{237}Np as well. Because the minimum lead time for the type of measurements and subsequent evaluation that are required is on the order of 5 years, it is important that the activities proposed here be initiated in the very near term so that the necessary information for the NGNP design in particular will be available in a timely manner.

In this portion of the planned INEEL NGNP R&D program, the INEEL, in partnership with Argonne National Laboratory (ANL) and various university and international collaborators, will conduct a collaborative research program to address the need for new nuclear data via the performance of measurements for the actinides of interest at the ANL Intense Pulsed Neutron Source (IPNS). Over the past several years, the INEEL Nuclear Physics Group has installed an array of detectors, the supporting electronics, and a data acquisition system based on techniques developed over the last two decades in nuclear physics at the IPNS, and has been using this array for the study of fundamental aspects of the nuclear fission process. This work and related previous work has produced over 100 refereed journal

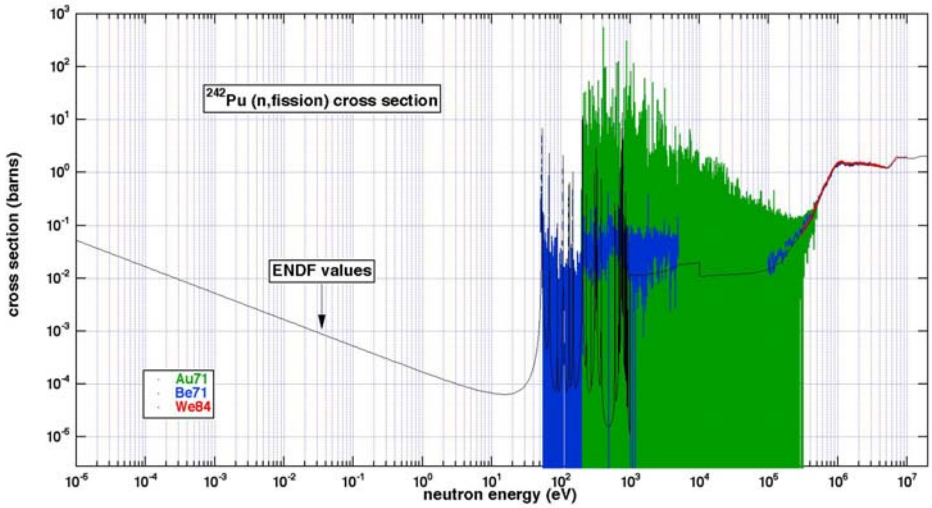


Figure 11. ENDF/B-VI data file values, black solid line, and available experimental data sets for the ^{242}Pu fission cross section.

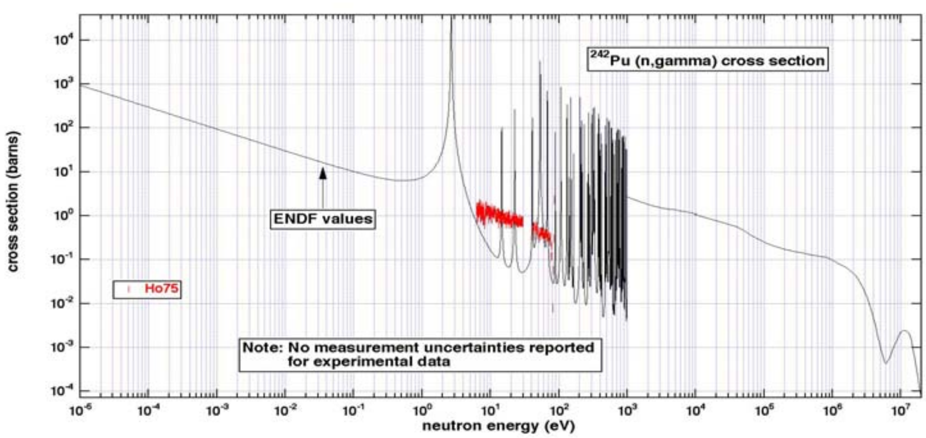


Figure 12. ENDF/B-VI data file values, black solid line, and available experimental data sets for the ^{242}Pu capture cross section.

papers over the years and it has established an international collaboration to support the experimental effort through data analysis. In the past year we have undertaken an effort to upgrade the system in a manner that will allow measurement of absolute nuclear cross sections as well, specifically to support this proposal. The proposed program will be coordinated with related efforts elsewhere, especially in the case of nuclear data measurements underway at the Los Alamos Neutron Science Center (LANSCE) under the Advanced Fuel Cycle (AFC) program. The work will complement, not duplicate, those efforts and it will result in substantial contributions to the national and international nuclear data base required to support the NGNP design in the near term and the overall Gen-IV advanced nuclear energy program in the longer term.

The detailed measurement of neutron-induced reactions was at one time the mainstay of nuclear research. That early work produced the extensive measurement data that exists for ^{235}U and ^{239}Pu, which were the isotopes of primary importance to the current generation of reactors. Since the early cross section measurement programs ended, instrumentation, experimental techniques, and computer-based data analysis have improved dramatically. These new techniques and the recent INEEL fission studies have led to a revitalized interest in this area. It is for example now possible to study the yields of the primary fragments that result from the fission process—in earlier experiments, this could only be investigated indirectly, by looking at the decay products of the prompt fragments after performing chemical separations.

Argonne National Laboratory's IPNS facility is one of the few accelerator-based neutron sources in the world where it is possible to do relevant neutron-induced measurements. The INEEL multi-detector measurement system at IPNS was used most recently to study information obtained from neutron-induced fission and capture reactions of ^{235}U, ^{239}Pu, and ^{237}Np. The experimental setup consists of an array of twelve Compton-suppressed high-purity germanium (CSHPGe) detectors and an array of eight liquid scintillation neutron detectors as shown in Figure 13. The detector array operates in coincidence mode, coupled to a dedicated data acquisition system designed for this application. The system collects data from a range of nuclear reactions concurrently, over the entire energy range covered within the limits of the timing parameters of the incident beam, which means that yields from several reaction channels ad all energies in the measurement range can be compared in an internally consistent way, without making several independent measurements. The different reactions are identified and extracted during the post-experiment analysis.

Through previous DOE direct funding and LDRD support, we have thus established the basic apparatus for an existing capability to measure neutron interaction cross sections at the ANL-IPNS facility. We plan to "fill gaps" in existing data and provide higher quality data over the neutron energy range of interest to the NGNP program, with a focus on fissionable isotopes of importance that were of minor interest previously. These will initially include the isotopes ^{237}Np, ^{240}Pu, and ^{242}Pu, with ^{241}Pu to follow closely thereafter. It is important to note that neptunium is included in the set of proposed measurements along with the plutonium isotopes of interest for several reasons. This isotope has been given a high priority by the AFC Physics Working Group in terms of the need for new nuclear data in

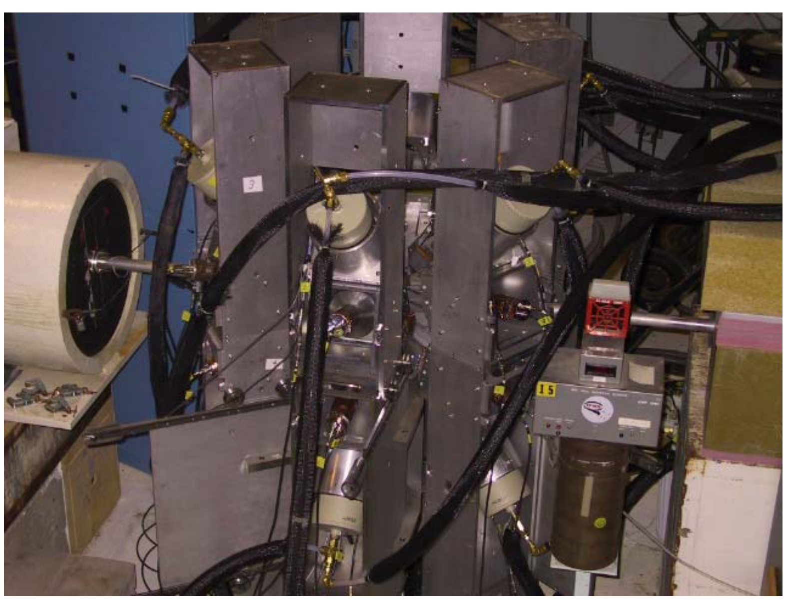


Figure 13. INEEL Detector array at ANL/IPNS.

connection with the AFC program, and some measurements for it are in fact currently being conducted at the LANSCE facility (Cappiello 2004). Although the need for new Np data is less for the NGNP, we have already completed an IPNS target design for this isotope and the necessary target can be made available in a shorter time frame than is the case for the Pu isotopes. Furthermore, and most importantly, initial measurements at IPNS for Np, by complementing the current measurements at LANSCE, will allow a cross calibration of the two independent experimental systems, not only improving the data for Np but also lending a greater degree of confidence in the subsequent Pu measurements. In addition, these cross-validation measurements will facilitate complimentary Pu measurements at LANSCE using targets fabricated originally for the planned measurements at IPNS, further improving the quality of the final data that ultimately will be entered into the ENDF evaluation process for these nuclides (see Capiello 2004).

Some initial reconfiguration activities for the INEEL apparatus at IPNS were conducted in FY-04 under LDRD funding and as noted below some NGNP funding was subsequently received in FY-04 for completion of the reconfiguration, thus laying the groundwork for readying a major resource for measurement of the needed cross sections. Plans have been made to acquire targets of the needed isotopes in the required form from the Federal State Unitary Enterprise "State Scientific Center Of The Russian Federation Research Institute Of Atomic Reactors" in Dimitrovgrad, Russia. This is an important aspect of the proposed work, since isotopically pure and metallic forms of the targets are not readily available in the United States. Also, an existing collaboration of university and national laboratory scientists in both the US and Russia exists to analyze and publish the results.

Workscope for FY-04: Initial NGNP funding in the amount of $238K was received in late FY-04 to continue the modification and refurbishment of the IPNS apparatus and to begin the Np and Pu target acquisition process. Subsequent to this, guidance was received from DOE restricting the use of this funding to preparation for, and responding to, a technical peer review of the IPNS protocol prior to beginning work. It is currently anticipated that this review will be completed by mid-October 2004. Thus the actual technical workscope would begin in early FY-05.

Workscope For FY-05: Calibration targets of ^{235}U are available on-site at ANL/IPNS for bringing the INEEL apparatus to a full operational level. These targets will be used with a new neutron flux monitor at IPNS to test and calibrate the system for both fission and capture measurements during the initial part of FY-05. This process involves encapsulating the uranium, testing the neutron flux monitor and its associated electronics, installation and testing of a new multi-stop time-digital converter currently being constructed under LDRD support, and collecting calibration data. Preparations would also be made to begin measurements for ^{237}Np.

Milestones for the initial part of FY-05 thus include testing of the neutron flux monitor, initiation of calibration measurements using the existing ^{235}U targets, finalization of the ^{237}Np target design in preparation for ordering, order this target, and initiating negotiations for suitable ^{240}Pu and ^{242}Pu targets from Russia.

The calibration with the uranium targets, as well as with some plutonium-239 targets available from another program, will continue until the arrival of the ^{237}Np targets. Analysis of the uranium data will be used to complete calibration and tests of the INEEL apparatus. With the neptunium targets installed and maintenance performed on the equipment, the neptunium measurements will become the experimental focus with a goal of ~3500 hours of neutron beam on target. In addition, a Gammasphere experiment (a passive radiation measurement using a sophisticated 4π detector array at ANL) will be requested for an existing but unique source of ^{240}Pu (currently on site at INEEL) for the background correction needed for the IPNS experiment measurements using that isotope. The ^{237}Np campaign, to begin in the latter half of FY-05 will require monthly system maintenance, calibrations with check sources and repair of the detectors during scheduled shutdowns of IPNS (annealing is routinely needed because of radiation damage). Analysis of data will be started with early checks to see that the apparatus is working correctly.

Milestones for the latter part of FY-05 will include completion of the uranium tests, initiation of neptunium measurements, and beginning the process for ordering the selected plutonium targets, ^{240}Pu and ^{242}Pu, with the order depending on schedule of availability. Deliverables for FY-05 will include monthly status reports of the experiment, the equipment, and operational results and any papers presented or accepted for publication.

Estimated costs for FY-05: $1230k

Workscope for FY-06: Complete neptunium measurements and begin analysis of the ^{237}Np data. During this year the detectors will be repaired (required due to neutron damage). Also analysis of the Gammasphere results will be done for corrections to the induced neutron measurements on ^{240}Pu. Complete procurement of plutonium targets. The plutonium measurements will then become the experimental focus with a goal of ~4000 hours of neutron beam on target. This will require continued routine maintenance, monthly calibration with check sources and repairing the detectors at the January and July, 2006 shutdown of IPNS. Analysis of plutonium data will be started with early checks prior to completion of the complete experiment, to verify that the apparatus is working correctly.

Milestones for FY-06 will include completion of neptunium measurements as well as completion of the plutonium target procurement process and initiation of measurements for ^{240}Pu. Deliverables for FY-06 will include monthly status reports of the experiment, the equipment, and operational results and any papers presented or accepted for publication.

Estimated costs for FY-06 are: $1255k

Workscope for FY-07: Complete ^{240}Pu measurements and begin analysis of the data. Deliverables for FY-07 will include monthly status reports of the experiment, the equipment, and operational results and any papers presented or accepted for publication.

Estimated costs for FY-07 are: $1415k

Workscope for FY-08: Initiate ^{242}Pu measurements early in the year and begin analysis of the data late in the year. Complete analysis of ^{240}Pu data. Deliverables for FY-08 will include monthly status reports of the experiment, the equipment, and operational results and any papers presented or accepted for publication.

Estimated costs for FY-08 are: $1455k

Workscope for FY-09: Complete ^{242}Pu data measurements and data analysis. Deliverables for FY-09 will include monthly status reports of the experiment, the equipment, and operational results and any papers presented or accepted for publication.

Estimated costs for FY-09 are: $1485k.

Workscope beyond FY-09 will be dependent on nuclide priorities set by the Gen-IV and AFCI physics working groups, but may include measurements of certain americium and curium isotopes of interest for potential advanced fuel cycles in the NGNP.

5. REACTOR KINETICS AND NEUTRONICS ANALYSIS DEVELOPMENT

The design of the NGNP requires the ability to carry out the following reactor physics design analyses: (1) static analysis for criticality and power distribution evaluations, (2) depletion analysis for core follow and effective fuel management, (3) dynamics calculations for simulations of transients and accidents, (4) heat deposition for thermal analysis, coolant flow allocation, and orifice design, (5) irradiation damage and shielding calculations for material performance and lifetime evaluations, (6) decay heat calculations for assessment of shutdown heat removal, and (7) sensitivity and uncertainty analysis to determine effects of data variations on reactor performance and safety characteristics. It is important to have a suite of computational capabilities that could meet these design needs.

Monte Carlo codes can be used for accurate prediction of the core characteristics of VHTRs, but they are still prohibitively expensive for use in extensive design calculations involving evaluation of local power distributions and small reactivity effects. Additionally, they do not provide all the capabilities indicated above. On the other hand, the deterministic code systems used for design and analysis of high-temperature gas cooled-reactors are generally based on older, less accurate methods that do not take advantage of advances in computer capabilities. These old codes have been superseded by more convenient and accurate capabilities. Modern deterministic tools have been developed in the last 20 years for LWR applications including assembly lattice codes, whole-core static and depletion analysis capabilities, spatial kinetics tools, etc. It is important to adopt these modern tools for the design and licensing of the NGNP, to improve accuracy, facilitate analysis, and meet modern quality standards.

Modifications of the available tools are, however, required to address the unique modeling issues of the NGNP core; additional heterogeneity due to coated fuel particles, neutron streaming in coolant channels, and power peaking problem at the core and reflector interface. In addition, they need to be integrated into a codes suite for NGNP applications. This integrated code needs to be verified and validated. Many of these issues are common to the pebble bed and prismatic designs. Development needs that are specific to one concept are identified as such and discussed in the following sections.

The work described herein begins the process of completing the suite of analysis methods to permit the full scope of NGNP design analysis calculations to be performed with state-of-the-art tools. An integral part of the development and testing of the new capabilities will be the assessment of their implications for design limits and margins. Thus, enhanced NGNP design and increased performance targets, improved passive safety goals, and improved non-proliferation characteristics for these reactors may be obtained.

5.1 Pebble Bed Reactors

Until recently, design analysis methods for pebble-bed reactors (PBRs) have been several generations behind the state of the art for light water design and analysis. For the past five years, the INEEL has been intently engaged in the development of analysis methods for PBRs. The laboratory has developed the PEBBED code for fuel cycle analysis and the PARFUME code for fuel materials analysis and is developing a method for quantifying material damage in graphite and silicon carbide reactor materials. A sample PEBBED graphical neutron flux output is shown in Figure 14. The availability of these tools has made possible innovations and discoveries that could not have been achieved without them. For example, the INEEL determined the reason for the success of the German TRISO fuel particles and the failure of other countries' fuel. Using a genetic algorithm developed to work in conjunction with PEBBED, the INEEL optimized design parameters to achieve passively safe PBRs of 600 MWt and greater. Using PEBBED, the INEEL was also able to propose design enhancements to the PBR that

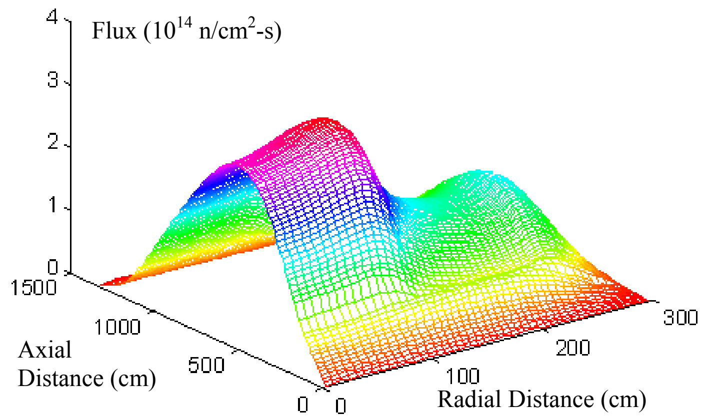


Figure 14. Thermal neutron flux profile in the NGNP 600 MWt reactor.

increased safety in water ingress accidents and improved fuel economy and utilization. All these significant design improvements were attained as incidental results of the verification of the new methods and the testing of their capabilities and the resulting extension of the design limits that can be reached.

The HTR-10 pebble bed reactor in the People's Republic of China can provide core physics benchmark data resulting from various startup core physics experiments. Since this problem involves no burnup dependence, the macroscopic group constants for fresh fuel compositions will be generated. Through the analysis of this benchmark, specific measures to improve the agreement with the experimental data will be examined. Effects of directional diffusion coefficients, nodal equivalence theory parameters to treat fuel/reflector couplings, and number of energy groups will be investigated. This analysis would demonstrate the adequacy of the nodal solutions.

One of the licensing issues for PBRs is the perception that the stochastic nature of the pebble distribution permits the collection of relatively reactive pebbles in regions of high neutron flux, so that the local power density could become excessive either in normal operation or in accident scenarios. Some rough estimates of the probabilities associated with this phenomenon were performed at the INEEL in 2003, indicating that the risks are very small. However, a more rigorous analysis is warranted and is possible with advanced Discrete Element techniques and other new modeling tools. Such tools can be used to develop flow models for pebbles in the discharge and entry regions and to examine pebble-packing issues.

5.2 Prismatic Reactors

Like that of the PBR, the knowledge base for the prismatic NGNP is limited to the data collected from a few operating high temperature gas reactors (DRAGON, Peach Bottom 1, Ft. St. Vrain) and the recent startup of a prototype facility in Japan (HTTR). Analysis methods and codes are generally decades old and, to some extent, not valid for NGNP applications. Double-heterogeneity, low-energy resonance treatment, graphite damage, and reflector lifetime are some of the issues that must be addressed for both concepts. Furthermore, options for block design are being considered that make physics analysis as challenging as that of the PBR.

High power peaking near the core-reflector interface necessitates changes to the block design in those regions. Some of the options that can be investigated include: using compacts with different enrichments or packing fractions, the use of burnable poisons, and modifying coolant channel geometry within the block. These necessarily impose demands upon the physics analyst to properly account for leakage effects, neutron streaming, and non-uniform depletion. Monte Carlo models can model these effects to a specified level of accuracy but the computational demands make codes like MCNP impractical for many design and sensitivity studies. Spectrum and assembly codes will require improvements to capture these effects in addition to those identified above.

The prismatic reactor uses batch-cycle fuel management as is the case with light water reactors. Thus, core simulator codes in existence can be applied with little modification to fuel cycle analysis as long as the cross sections are generated properly. The fuel and reflector blocks are right hexagonal prisms and thus an established hexagonal code is well suited for this geometry. DIF3D-REBUS (Derstine 1984; Lawrence 1983; Palmiotti et al 1995; Toppel 1983), developed at ANL for fast reactor cycle analysis, will be analyzed to see what modifications may be required to enable its use for NGNP.

Complicating the matter to some extent is a proposal for axial and radial reshuffling of fuel blocks. Axial reshuffling leads to better fuel economy and lower fuel stress as is the case with the PBR but will require a powerful fuel management code. Sophisticated core optimization techniques have been applied successfully to light water reactors (and recently to the PBR) but have yet to be applied to the prismatic core. Radial reshuffling will also be complicated if new block designs involve non-uniform fuel loading and burnable poisons. Development and application of modern core design tools will be required in order for block core designs to achieve NGNP technical specifications.

5.3 Neutron Diffusion and Isotope Depletion Methods

Implement Analytical Nodal Algorithms in Core Simulator Codes. PEBBED's two and three dimensional diffusion solver is based upon a standard finite difference algorithm. This method is not efficient for extensive design optimization. Work is underway to implement an analytical nodal solver in cylindrical coordinates developed at the INEEL as part of an LDRD project. The solver has been successfully demonstrated for one-dimensional problems. Once fully implemented, the diffusion solver will yield a highly efficient and accurate code for all PBR calculations.

The DIF3D/REBUS-3 code system is capable of multigroup flux and depletion calculations in hexagonal-Z geometry. This code system uses the DIF3D module as the flux solver and contains both nodal diffusion and transport theory capabilities. Therefore, it can be adapted to prismatic NGNP reactor problems with limited effort compared to other codes. Some enhancements will be implemented to exploit recent developments and the results of this NGNP research effort.

Reactor kinetics studies require calculations of kinetic parameters such as delayed neutron fractions. These are generally obtained from adjoint flux calculations on the core model. DIF3D possesses adjoint capability but PEBBED currently does not. The analytic nodal equations will be modified to allow for an adjoint solution and the solver in PEBBED will be upgraded.

Nodal depletion solvers offer improved accuracy over other approaches. An analytical nodal depletion solver using a "moments-stepping" method that allows for variable cross sections within nodes has been developed by an INEEL researcher. The new method will be implemented in the pebble-bed and prismatic codes.

Detailed power deposition taking into account transport of gamma rays is necessary for thermal calculations, coolant flow allocation and orifice design, and the simulation of irradiation behavior of the graphite block. This calculation requires that gamma production and transport in the core be accurately calculated. The DIF3D/GAMSOR calculational path will be evaluated and modified for use in the NGNP analysis.

PEBBED possesses an advanced optimization routine (a genetic algorithm) that allows automated searches for optimal core designs and fuel loading patterns. An equivalent feature does not exist in DIF3D. Light water reactors also have benefited by the application of different advanced optimization schemes for fuel reload analysis. Such a tool has yet to be developed for the prismatic reactor but is needed because of the numerous degrees of freedom being proposed for the prismatic NGNP. Fuel blocks are proposed that may have compacts with differing enrichments, packing fractions, and burnable poison concentrations. The block refueling pattern may be strictly radial or may have an axial shuffling component as well. Core optimization and fuel loading must be automated to some extent to produce viable cores within practical time limits. There are a number of advanced optimization approaches including: genetic algorithms, simulated annealing, neural networks, Tabu search, and others. One or more of these will be explored and implemented in DIF3D/REBUS.

The work required to achieve these objectives is listed in Figure 15 and the time line of each task is shown. The total cost of the neutron diffusion and isotope depletion methods work scope is $1,075k.

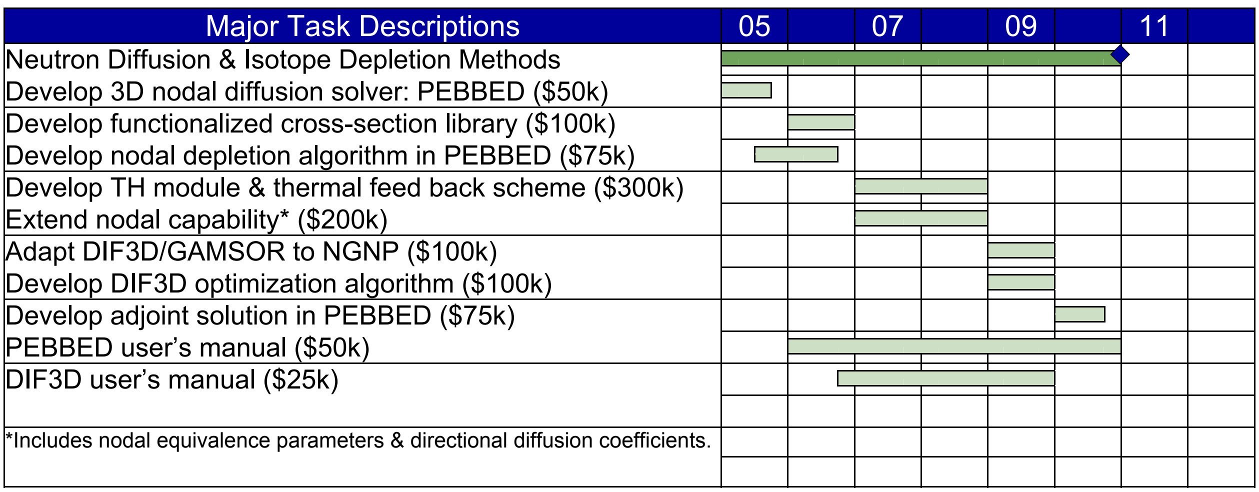


Figure 15. Timelines and estimated costs of neutron diffusion and isotope depletion methods R&D.

5.4 Spectrum and Cross Section Generation

Modify A Cross-Section Generation Code To Treat Low-Energy Resonances With Upscattering. Cross sections used by PEBBED are currently calculated externally and passed to PEBBED as input. Initially, these cross sections were calculated by the INEEL's COMBINE code. However, COMBINE does not account for resonances in the thermal energy range in graphite-moderated reactors where upscattering is significant. This omission matters little for light-water reactors or for low-burnup graphite-moderated reactors, but it leads to substantial errors in the harder spectrum of a graphite-moderated reactor when high burnup is sought. In subsequent work, COMBINE was replaced by MICROX-2, which was specifically devised for gas-cooled, graphite-moderated reactors. However, the proper use of MICROX requires a specially produced library to be generated with a known standard version of the NJOY code. In addition, other possible deficiencies have been identified as needing R&D.

In addition to the deficiency addressed above, there is sketchy evidence that the low-energy resonances that become important in high-burnup fuel (see Figure 16) may be treated incorrectly by existing codes because all of the usual simplifying assumptions of resonance integral theory are not applicable. Hence the required R&D must determine whether a rigorous treatment of the low-lying resonances is indeed present in the codes available to the INEEL. If not present, code corrections will be required and the corrections will be implemented either in the existing codes or in a separate stand-alone code. This can be achieved by over-writing the thermal cross-sections with properly self-shielded cross-sections that account properly for all of the resonances in an algorithm that sweeps through the thermal groups to update the upscattering source terms. A group-wise (rather than a point-wise) thermal spectrum calculation must be implemented in this case. Both COMBINE and MICROX would require this modification.

The modifications to any of these codes could be construed as forming the basis for a future DOE-owned standalone modern code for a proper treatment of resonances.

Develop A Method For Double Heterogeneity Treatment Using Improved Dancoff Factors. Many codes used for gas reactor analysis were developed without a full appreciation of the importance of randomness in particle distribution. Calculations at Georgia Tech indicate the error introduced by assuming a regular array of fuel lumps (Table 6). Similarly, COMBINE does not give acceptable agreement with continuous-energy MCNP calculations. (However, MCNP is not applicable by itself to anything but a fresh-core PBR, as it cannot account for fuel motion and the development of an asymptotic steady-state burnup distribution, whereas PEBBED was written precisely to do this.) Before accurate cross sections can be calculated for use by PEBBED, either COMBINE or MICROX-2 must be modified, or a whole new cross section processing code must be written. This work has begun at the INEEL.

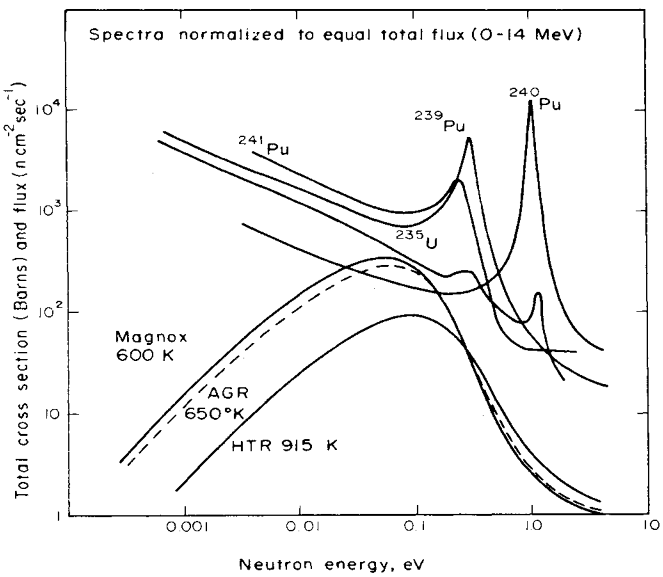


Figure 16. Typical HTGR spectrum and some low-lying resonances.

Table 6. Differences in k_{inf} between MCNP and DRAGON (ANL).

Computation model	NGNP, $UC_{0.5}O_{1.5}$
Stochastic average	1.53280 ± 0.00082
DRAGON	1.54393 (0.73%Δk/k)

An important aspect of improving cross sections is to account better for the heterogeneity on two scales in the NGNP: on the fine scale, from the fuel particles, and on the coarse scale, from the pebbles or fuel compacts. For the PBR, self-shielding and shadowing effects are important and must be accounted for on both scales. In the continuous-energy Monte Carlo code MCNP, it is possible to model every single fuel grain in the reactor, using the repeated structures feature. However, in deterministic codes like PEBBED or DIF3D, these features are accounted for in the cross sections they receive as input. Such cross sections must be generated using explicit modeling of the heterogeneity or using correcting factors that account for it (the Dancoff factors). Previous studies show that the available Dancoff factors are not sufficiently accurate. Hence the new method must also include accurate corrections for the effects of double heterogeneity.

Other improvements to the COMBINE code that would greatly improve its accuracy and effectiveness for NGNP analysis have been identified by INEEL developers in the early stages of a spectrum code assessment.

With the advent of ENDF/B-6, the basic strategy adopted for COMBINE was to use NJOY as the processing code for a 72-group fast cross section library and a 101-group thermal cross section library. The standard NJOY output for resonance self-shielding is a set of Bondarenko multigroup data as a function of temperature and background dilution cross-section. In addition to the standard Bondarenko multigroup data representation in the epithermal energy range, a separate library is generated for the resolved resonance parameters directly extracted from ENDF/B-6 over an arbitrary energy range. The Bondarenko method is basically an "infinite medium" method that parameterizes cross sections for a nuclide as a function of temperature, T, and the "background dilution" cross section, σ_0, of all the other nuclides mixed with the nuclide. Simplistically, given the temperature and background dilution cross-section values, one determines self-shielded cross-sections by interpolating in tables. Since self-shielding causes the "background dilution" values that a nuclide sets to change, an iterative procedure involving all nuclides is used. To account for two region systems, the σ_0 value is augmented by an escape cross section, σ_e. This escape cross-section value is a function of the total cross-section value in the medium and its geometry.

Multizone situations, such as reactor lattices, are accounted for by the use of Dancoff factors, which, in effect, modify the escape probability and, hence, the value of σ_e. To better account for the double heterogeneity due to fuel grains present within the macroscopic fuel lump, a correction is made to the escape probability. The accuracy to which resonance parameters are computed depends directly upon the validity of the Dancoff factors.

In a resolved resonance region, a more accurate Nordheim Integral Treatment is used. This treatment involves a solution for the energy dependence of the neutron flux in a material region containing a resonance absorber and a maximum of four admixed moderators. The material region may be infinite in extent or it may correspond to a 1-D slab, cylinder, or sphere surrounded by a moderating medium in which the neutron flux is spatially flat and varies slowly with energy. The presence of more than one absorber lump in the moderating medium (e.g., a fuel pin lattice or randomly dispersed kernels) is again accounted for through the use of a Dancoff factor. The Nordheim treatment is generally more precise than the Bondarenko method in the resolved resonance region and will be implemented in the chosen spectrum code. Other minor improvements that will yield benefits for NGNP analysis include:

- Energy dependent bucklings for more accurate leakage corrections
- Improvements in the transport correction to diffusion code parameters
- Added capability of processing Adler-Adler and Hybrid R-function resolved resonance formats
- Inclusion of g-, f-, and d-wave as well as p- and s-wave levels in the resolved resonance parameters.

A PBR can operate with very little excess reactivity at normal operating temperature; however, as the temperature decreases, reactivity increases because of the increased resonance escape probability (the

Doppler effect for temperature decrease). At cold shutdown temperatures, some control rod insertion is required to keep the reactor from restarting itself. Control rods are also required to shut the reactor down rapidly on demand. For the prismatic core analysis, DIF3D contains a variational transport solver that can properly treat regions in which diffusion theory is not valid. Work is underway at Georgia Tech and the INEEL to develop transport methods for treating control rod and void regions in pebble-bed reactors. These methods will be incorporated into PEBBED.

The fission process produces a large assortment of fission-product nuclides, and it is customary in light-water reactor (LWR) analysis to lump them all for convenience into a generic fission product pseudonuclide. However, no such pseudonuclide has been generated for the spectrum in graphite-moderated reactors. One or more lumped fission products suitable for NGNP analysis will be generated as part of this effort.

Identify or Develop an Assembly Code for Prismatic Block Cross-Section Generation. The prismatic reactor core is composed of hexagonal graphite blocks containing coolant channels and fuel compacts. The compacts contain TRISO particles distributed randomly within. The core simulator code such as DIF3D has as its basic computational element a hexagonal cell for which few-group diffusion coefficients must be computed by a lattice or assembly code. Previous analyses indicate that an under-prediction of more than 3% in the k-infinity of a fuel pebble can occur if the fuel-graphite composite is treated as a homogenized mixture. Therefore, the lattice transport code to be used for group constant generation must be able to treat the double heterogeneity properly. This capability is available in a few lattice physics codes such as WIMS, APOLLO2, DELIGHT, and DRAGON. Where such capabilities exist, the codes (e.g., WIMS8 and APOLLO) are typically proprietary and are only available at great cost. In some cases, the source code is not available for release. This makes the DRAGON code attractive and for this reason it will be evaluated as part of this project. (The code is being developed by researchers at the Ecole de Polytechnique in Montreal). Some members of this research team worked on the APOLLO code. The DRAGON code capabilities and models that are relevant to the NGNP will be evaluated. The effort will focus on the double heterogeneity and resonance treatments for coated fuel particles, the best format for the cross section data library (DRAGON does not come with own library), transmutation and decay chains, modularity of code for staged calculations, and code performance compared to those of higher fidelity models/codes (e.g., Monte Carlo simulations – see Figure 17).

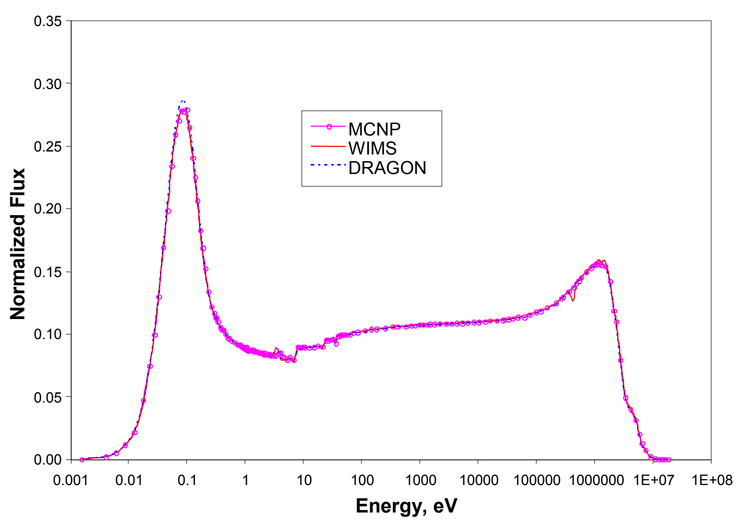


Figure 17. Comparison of VHTR spectra generated by various codes (ANL).

To devise an appropriate functionalization scheme, the dependencies of cross sections of the NGNP fuel block on various state variables will be investigated using results of the DRAGON and WIMS8 lattice codes. It is noted that the planned code suite is not limited to the use of these two codes for cross section generation. Other lattice codes can be plugged later in this code suite, once their performance for VHTR analyses has proven to be satisfactory.

A group constant processing code will be written that automates the process of generating homogenized multigroup cross sections for the fuel, reflector and control blocks as a function of state variables. Nodal equivalence theory parameters and directional diffusion coefficients will also be generated to account for the homogenization errors expected in the regions where significant material discontinuities exist. Examples of these regions are the core/reflector interface and control rod regions. A group constant functionalization scheme will also be developed and implemented in the group constant processing code. Both table lookup and polynomial fitting approaches will be considered.

A complete assessment of code deficiencies and necessary modifications that would make the code attractive for NGNP applications will be provided. This effort will require interaction with the DRAGON team, since it is also intended to obtain better code documentation, support for alternative data library, and descriptions of advanced models and capabilities not in public domain (e.g., methods of characteristics solution, homogenization/de-homogenization, parallel code version).

The work required to achieve these objectives is listed in Figure 18 and the time line of each task is shown. The total cost of the spectrum and cross-section generation work scope is $1,375k.

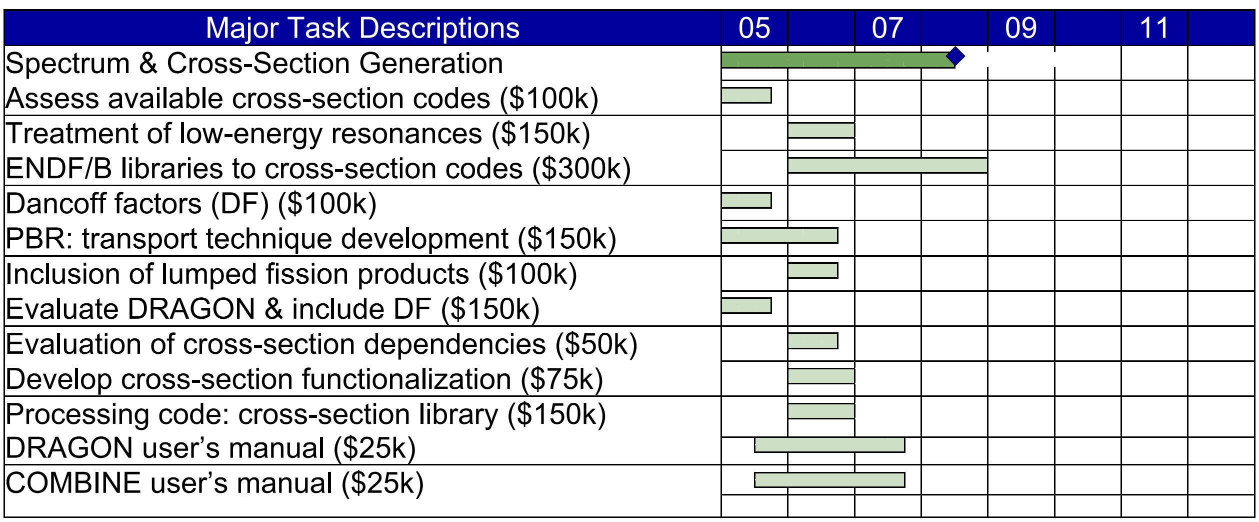


Figure 18. Timeline for spectrum and cross-section generation R&D.

5.5 Kinetics, Thermal Module Coupling, and Feedback

Perform Quality Assessment On Thermal-Hydraulics Code. Thermal-hydraulics calculations are an important part of the safety analysis of the NGNP. Validation of the appropriate thermal-hydraulics tools is required for their use in these calculations. PEBBED possesses simple thermal-hydraulic models for estimating core temperatures. While these allow for rapid scoping and design optimization, they are unlikely to yield accurate thermal-hydraulic data. Assessment of various thermal-hydraulic codes and comparison to PEBBED results are required to identify areas of need.

There are three candidate thermal-hydraulics codes. One of these is the INEEL's RELAP5/SCDAP suite of codes, and another is the INEEL's version of MELCOR. For several years, the INEEL has been using MELCOR for PBR safety analysis, because it is able to model transport of the dust released by inter-pebble contact; the INEEL's version can also treat air and water ingress and helium coolant flow. However, these capabilities have recently been added to RELAP5/SCDAP, so it is not clear which of these codes is now better suited overall to model PBR safety problems. The third code is ORNL's GRSAC code, which was specifically written for gas-cooled reactors. A comparison will be made, and the chosen code will be validated for NGNP design applications.

As a first step to improved PBR design, the THERMIX two-dimensional gas reactor thermal-hydraulics code has been acquired and coupled to PEBBED. THERMIX improves PEBBED calculations of steady-state thermal-hydraulic conditions and depressurize loss of coolant (DLOFC) transients. Benchmarking efforts must be completed.

A relatively large coolant pressure drop through the pebble field is one of the few disadvantages of the PBR compared to the prismatic-fuel NGNP. A Japanese team has recently shown that radial coolant flow reduces these pressure losses so much that the pressure drop advantage can actually go to the PBR. Thermal-hydraulic tools must be adapted to model radial flow of coolant.

Kinetics Development. Three-dimensional, spatial kinetics capabilities have been under development for more than 20 years. Practical tools now exist and include the public versions of NESTLE, PARCS, VARIANT-K, and DIF3DK. These high fidelity kinetics methods are important for core transients involving significant variations of the flux shape but have not been systematically applied to graphite-moderated, helium-cooled reactors. In the future, integrated thermal-hydraulic and neutronic methods should be extended to enable modeling a wider range of transients pertinent to the NGNP. Required advances include increasing the efficiency of the coupling approaches and improving the representation of cross section variations. Developmental steps should begin with existing tools as follows.

The work applicable to PBRs would begin with the extraction from PEBBED of the portion of the code that solves the neutron diffusion equation. This has already been done for an earlier version of PEBBED, which did not contain the nodal solution option. The present work would include the nodal solver.

The diffusion equation solver that would be extracted from PEBBED would be general – i.e., it would contain a fission term in the source. The fission source is calculated in an "outer iteration" as typically done in reactor physics analysis. For the purposes of this project, it will be necessary to extract the "fixed-source solver" from this general solution code.

Next, time-dependence must be introduced into the fixed-source solver and the source term reformulated to account separately for prompt and delayed neutrons, for neutron kinetics analysis within a PBR systems model for a code such as RELAP5.

Kinetics is the study of very short-term transients in the neutron flux, so it is not necessary to account for the motion of the fuel in kinetics analyses. The portions of PEBBED that account for fuel motion (the burnup equation solver and the pebble recirculation matrix) are not needed for kinetics calculations, and it would unnecessarily encumber RELAP5 to couple it to the full PEBBED code.

Initially, the time-dependence in the kinetic equation will be treated with finite-difference techniques, but once this method is working more advanced approaches to treating time dependence will be explored. One promising approach that will be investigated is that of starting from the P1 equations (without the assumption of a non-varying current) and to solve analytically (or semi-analytically) the coupled flux and current equations. It is possible in this way to relax most of the assumptions made in the derivation of neutronic kinetic computational schemes.

Nodal diffusion and transport kinetics capabilities have been developed for the DIF3D code in the past. These capabilities have been successfully applied for transient analysis of thermal reactor systems (e.g., NPR-HWR, RMBK, VVER, and LWR), by integrating in a system analysis code, SASSYS. Initial estimation indicated that a multigroup analysis (about 20 groups) is required to represent accurately the reactivity effect due to spectral change. The multigroup capability of DIF3D would be attractive for integration with a system code, such as RELAP5/ATHENA, that can be utilized for the analysis of the NGNP. Eventually, it can be upgraded with the new kinetics treatment described above.

Annealing Feedback. Thermal feedback is usually accounted for in traditional neutron kinetic codes that are suitable for the analysis of light water reactors. Other forms of feedback are unimportant and are not explicitly modeled. For the NGNP, the situation could be drastically different. Of particular importance is the change in material properties caused by radiation. For example, the thermal conductivity of graphite is degraded gradually as radiation damage accumulates. Similarly, some nuclear properties, such as the scattering cross sections are altered by the irradiation damage. During transients, the increase in temperature may anneal some or all of the damage, resulting in (partial) property recovery. This could, for example, imply that the scattering cross section would increase during a transient, resulting in stronger thermalization properties and an increase in reactivity. Other similar phenomena are believed to occur that also have a potential impact on the safety of the NGNP during extreme transients. The feedback mechanisms just described must be incorporated into the kinetics codes. This will require their correct modeling and then the incorporation of said modeling into FORTRAN code. The characterization of irradiation damage and its effects on material, neutronic, and thermal properties is another task in this research.

The work required to achieve these objectives is listed in Figure 19 and the time line of each task is shown. The total cost of the kinetics, thermal module coupling, and feedback work scope is $1,225k.

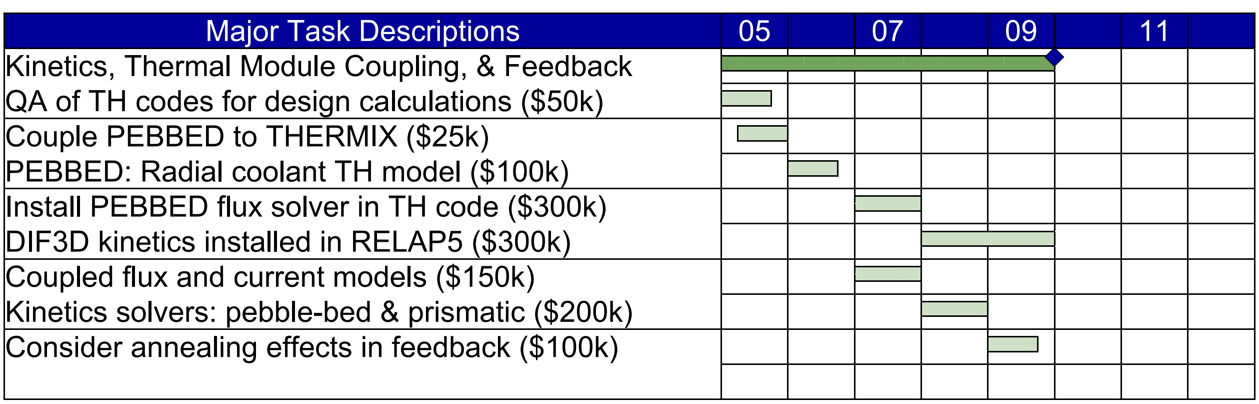


Figure 19. Timeline for kinetics, thermal module coupling, and feedback.

5.6 Pebble-bed Core Modeling and Effects

Approach to Asymptotic. PEBBED obtains the asymptotic distributions of neutron flux and burnup directly, without following the time-dependent distributions in the run-in period. This property of the code permits very rapid solution. However, there are situations where it is desirable to follow the time-dependent development of the asymptotic solution. In previous work, a method has been formulated for obtaining the time-dependent solution for the neutron flux and burnup distributions during the run-in period. In this task, that solution will be implemented in PEBBED and time-dependent solutions of the coupled pebble-flow/burnup problem will be found. This task is divided into two main parts. In the first part the method will be elaborated and coded for a single axial depletion zone within the reactor core (i.e., single coarse node). The resulting method will apply directly to an entire core if it is assumed that the flow of pebbles is strictly axial.

Non-Axial Pebble Flow. The flow of pebbles in a PBR is not strictly axial. A method and code are to be developed that link together depletion zones along the true flow path of pebbles even for flow lines that are not strictly axial. In this development the axial flow of pebbles is modeled, as in the previous case. In addition, the radial drift of pebbles is also accounted for. Effective pebble flow characteristics are developed and used to link computational coarse nodes systematically.

The behavior of pebbles in the outlet of the bottom of the vat deserves careful attention (see Figure 20). The rate of pebble removal will be on the order of 0.1 per second, so that pebbles will pass through the outlet one at a time. This low flow rate implies a narrow throat, which in turn may create a bridging phenomenon in which a cavity develops periodically at the outlet, to be filled abruptly as the bridge above it collapses. This collapse could of itself induce an increase in the overall packing fraction in the vat, with the associated reactivity transient.

***Variable Pebble Packing and Slumping*:** Experiments relevant to the PBR have shown that the average packing fraction of pebbles in the vat is expected to be about 61%, but that in the presence of shaking (such as may occur during an earthquake), the packing fraction may increase to as much as 64%. The PIs of this proposal have done calculations to show that an increase of packing fraction from 61% to 64% may cause significant "reactivity transients" (i.e., power surges) in a PBR.

Furthermore, the packing is not uniform. The packing fraction is exactly zero at solid walls and approaches an asymptotic value through a series of spatial oscillations over a distance of several pebble diameters. In a PBR, such a distance may be a significant portion (e.g., 20% or more) of the vat radius. If the vat is surrounded by a neutron reflector, as it probably will be, these fluctuations occur in a region of high thermal neutron flux, so that the fluctuations will have exaggerated importance.

The rigorous prediction of pebble packing and flow behavior is important for purposes of PBR safety analysis and licensing, as well as for predicting spatial and temporal power fluctuations in normal operation. Proper evaluation of these effects requires the analysis of pebble flow through a cylinder or annulus. Discrete element techniques and codes exist and have been applied to the modeling of pebble-bed cores (Figure 20). This analysis will be applied to the problems of hotspot formation, pebble-packing variation, pebble-bed slumping, and pebble flow near discharge tubes.

The work required to achieve these objectives is listed in Figure 21 and the time line of each task is shown. The total cost of pebble-bed core modeling and effects work scope is $600k.

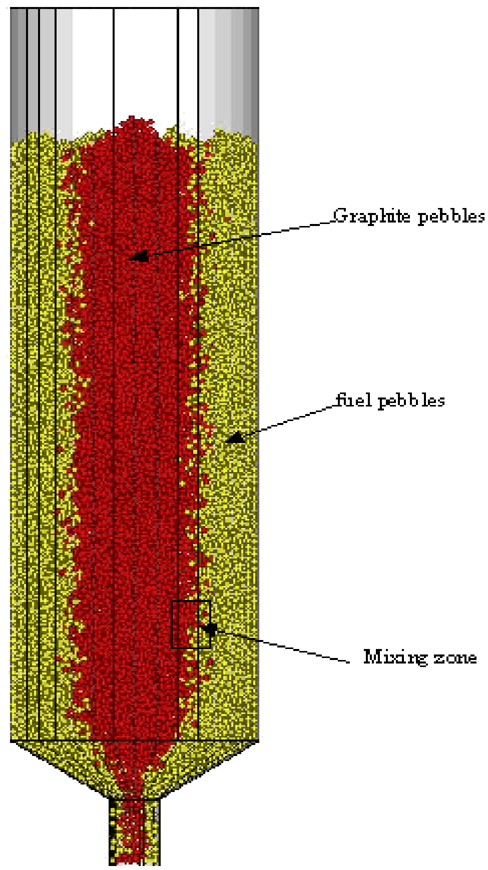


Figure 20. Discrete element representation of a two-zone PBR.

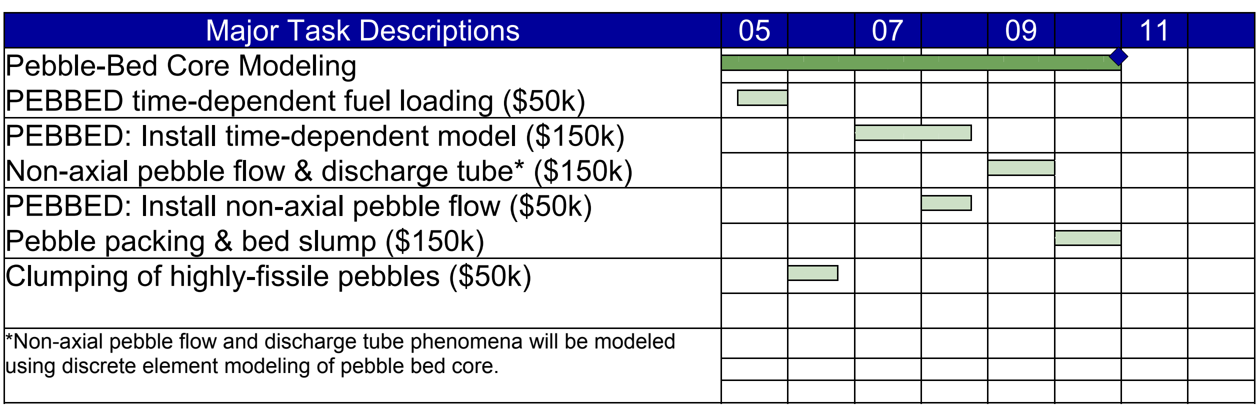


Figure 21. Timeline of pebble-bed core modeling R&D.

5.7 Kernel Design, Irradiation Damage and Annealing Effects

Optimize Kernel Size And Packing Fraction. One design issue that will be studied as the new tools are developed is the diameter of the fuel kernel within the TRISO particle. Changes in this parameter (while otherwise maintaining the overall TRISO structure and overall diameter) are expected to have profound effects on fuel burnup, fission product migration, and fuel particle reliability. This task will support the final fuel particle design selection.

Develop Improved Methods For Calculating Material Damage From Irradiation. The primary mechanism for material damage by neutron irradiation is atomic displacement. The threshold energy E_d for this displacement depends strongly on temperature, yet methods to account for this dependence have not been developed. The INEEL has recently developed a state-of-the-art method to estimate displacement damage cross sections in many materials of interest in the Generation IV program. Consequently, R&D during this year will focus on obtaining improved estimates of E_d, including temperature dependence, for use in the new INEEL method. Furthermore, radiation damage in high-temperature materials can be annealed by the effects of heating and by further irradiation. A second goal of this task is to account for these annealing processes in the INEEL material damage model. This task is very complex and brings into play many areas of physics and computational science. For example it requires a thorough understanding of the inter-atomic potentials in the solids under consideration and the dynamics of collisions in these materials. The proper modeling of the displacement threshold will require the incorporation of thermal motion and its impact on effective average inter-atomic potentials. Also to be incorporated is the modeling of collisions and atomic rearrangements, taking into account return to location of origin or to equivalent locations as affected by thermal motion. Because of the level of complication, this task will require a multi-year effort. Initially, the inter-atomic potentials for the materials of interest will be researched and the modeling requirements stemming from their changes because of temperature will be assessed. Later on, a new computer code will be written or an existing one will be modified to incorporate thermal motion into the modeling of collisions and subsequent atomic motions and settling in new lattice positions. Annealing will also be modeled toward the end of the task. To limit this task to a manageable size it is understood that the methods to be developed will target one or two materials at most. The principal material to be addressed will be graphite. In addition, silicon carbide (SiC) will be considered if time permits and data and suitable inter-atomic potentials can be obtained.

Graphite and silicon carbide (SiC) are key materials in the development of Generation IV reactors. Graphite is the moderator in both the prismatic and pebble bed designs of the Very High Temperature Reactor (VHTR) concept. SiC is used as the coating material for the TRISO fuel that is a candidate for use in the VHTR and possibly the gas cooled fast reactor (GFR). In the harsh reactor environment (intense neutron flux, high temperature, etc.), materials will suffer from atomic displacements (radiation damage) that are initiated by the interacting neutron field. These displacements are generally accepted as the underlying causes for many macroscopic manifestations (radiation effects).

The estimation of the number of displacements in a given neutron field requires knowledge of the displacement threshold energy (E_d), i.e., the lowest amount of energy that could cause an irreversible displacement if imparted to an atom in a solid. In general, E_d is expected to depend on the direction of motion in a crystal. This is due to the fact that E_d may be viewed to represent the minimum energy needed to cross the potential barrier that surrounds an atom. However, because of the nature of crystallographic structure, the potential barrier may not be isotropic, which introduces variation in the threshold energy needed to overcome it. Furthermore, graphite related experiments did show that E_d in graphite depends on direction. In addition, computational simulations for SiC revealed a similar dependence for E_d on crystallographic direction. On the other hand, the possibility does exist for E_d to also depend on the temperature of the material. In fact, experimental evidence for graphite show such dependence. Nevertheless, most experimental determinations of E_d are conducted at temperatures close to room temperature, whereas models also assume a low temperature (often essentially 0 K). For most applications, this is acceptable. However, for applications related to reactors such as the NGNP, the values of Ed determined at 0 K or at room temperature may not be adequate. In this project, the values of E_d for graphite and SiC will be determined as a function of direction and at temperatures representative of those of the structural materials and of the fuel in the NGNP.

In addition to the above, it is well recognized that the accumulation of damage in graphite manifests itself in increasing the stored energy. If stable damage formations are created at the operating temperatures of the VHTR/NGNP, then unplanned/unexpected increases in temperature (transients) could result in the release of this energy and the potential creation of a positive feedback situation. To estimate the impact of this effect on reactor safety and operational characteristics, it is essential to determine its time behavior. Clearly, effects characterized by long time constants (i.e., slow effects) will be easier to remedy than prompt effects that are characterized by extremely short time constants.

The needed studies in this work can be performed using classical molecular dynamics (MD) simulations running on parallel computers. At the heart of the MD simulation is the choice of the potential function. The gradient of this function with respect to atomic displacement determines the forces on each atom. The integration of the equations of motion of the interacting particles yields the trajectory information. Consequently, the choice of the appropriate potential function is essential for the fidelity of the simulation. In general, many body potentials are used to describe materials such as metals and semiconductors and a few have been used for graphite. In addition, it is possible that potential functions can be constructed using ab initio (i.e., first principle) quantum mechanical simulations and subsequently used in the MD calculations. These options will be explored in this work.

The design and the operational life of some structures in the NGNP reactor are limited by the material properties of graphite. Under irradiation many properties of graphite change. The estimation of these changes as the reactor is operated well into the future requires the availability of means to estimate the accumulation of damage. This is routinely done by estimating the displacements per atom (dpa) in the material. Tabulation of the appropriate displacement kerma cross sections will require the availability of temperature-dependent estimates of the displacement threshold energies. This project will yield such threshold energies. If high-temperature energy releases are feasible, then their temporal dependence must be accounted for in safety simulations. In particular, the analyses that rely on the current definition of passive safety (generally accepted for NGNP reactor designs) may have to be revisited. Indeed, currently a design is considered passively safe against transients if by passive means the fuel temperature is made to remain below about 1600 °C during all transients, regardless of severity. This temperature may be above that at which the high temperature release is suspected to occur (between 1200 and 1500 °C). If this energy release is slow then it would allow for intervention. While a prompt energy release may require a revision of the safety analysis of for this type of reactor.

The work required to achieve these objectives is listed in Figure 22 and the time line of each task is shown. The total cost of kernal design, irradiation damage, and annealing effects work scope is $300k.

Major Task Descriptions	05		07		09		11	
Kernal Design, Irradiation Damage, & Annealing								
Relate kernal size effects to core design ($50k)								
Molecular dynamics model ($50k)								
Evaluate existing potential functions ($50k)								
High temperature energy release* ($50k)								
Calculation of displacement energy as function of temperature: generate displacement kerma cross-sections ($100k)								
*High temperature energy release as function of time—evaluate effects on reactor safety								

Figure 22. Timeline for kernal design, irradiation damage, and annealing.

5.8 Improvement, Validation, and Verification (V&V) of Code Suite

The resulting suite of deterministic codes developed above will be verified against Monte Carlo and deterministic codes and against integral experiments. The double heterogeneity treatment will be examined for detailed fuel block and pebble problems by comparing the lattice code solutions with continuous energy Monte Carlo solutions. The whole-core solution scheme will be verified against multi-group Monte Carlo solutions using pre-calculated multi-group cross sections and homogenized fuel-element models. The PBR solution will also be compared against VSOP results.

After all the improvements and the extensions are completed, the overall accuracy of the suite of codes will be quantified by analyzing appropriate integral physics experiments. All known reactors, critical facilities, and other experiments of both types have been assessed for suitability as benchmarks. For the prismatic reactor, the HTTR facility in Japan possesses large amounts of critical reactor physics data that can be used for validation purposes. For the pebble bed reactor, the HTR-10 or AVR may also provide critical data. At least one of these will be the one selected for a full evaluation under the integral benchmark data task (see Section 4.2). Additional validation tests will be performed using available experiment data from past and existing facilities such as the Proteus and ASTRA experiments.

V&V of the tools used for these predictions can be met through the collection of a large compendium of relevant in-core critical experiment data into a detailed, peer-reviewed standard format. Such an approach has been taken by the USDOE-NNSA in handling V&V for stockpile stewardship, where computer modeling is also relied upon extensively. In support of this effort, it might be necessary to establish and promulgate V&V standards or at least some set of test problems for Generation IV systems. If suitable validation and verification data do not exist, experiments will have to be designed and conducted to fill in the gaps. This task is covered in the previous chapter.

Monte Carlo simulation itself provides a powerful tool for validation and verification. The recent and continuing growth in computer power motivate the assessment and further development of Monte Carlo-based analysis capabilities applicable to multiple reactor types. Enhancement of these codes would also be investigated, including the propagation of errors as a function of depletion, provision of temperature interpolation capability, and modeling of thermal-hydraulic feedback.

The 3-D whole-core transport code DeCART is being developed based on the method of characteristics for LWR applications at KAERI under an ongoing I-NERI project. This code eliminates the approximations and laborious multi-group constant generation stage of the two-step approach by representing local heterogeneity explicitly without homogenization, using a multi-group cross section library directly without group condensation, and incorporating pin-wise thermal-hydraulic feedback. With the extension of the geometry handling capability and the inclusion of double heterogeneity treatment, this code could be used as the reference tool for verifying and validating the nodal codes along with the partial use of the Monte Carlo solutions. The DeCART code could also be used as a lattice physics code for generating group constants. Thus it would have the dual functionality of group constant generation and whole-core calculation. An adaptation of the DeCART code for VHTR analyses will be pursued under a new I-NERI collaboration with KAERI. This will leverage the U.S. cost for this effort.

The required enhancements to the initial suite of codes identified by the validation and verification effort will be implemented. This activity will be continuous and is tied to the validation and verification effort.

Sensitivity and uncertainties (S&U) activities, complementary to the S&U activities specific to nuclear data (see Section 4.1) will be performed for computational capabilities. S&U activities will be ongoing until fiscal year 2013.

Finally, the U.S. Nuclear Regulatory Commission (USNRC) will be included as an independent reviewer regarding the qualification of codes.

The work required to achieve these objectives is listed in Figure 23 and the time line of each task is shown. The total cost of improvement, V&V of code suite effects work scope is $4,000k.

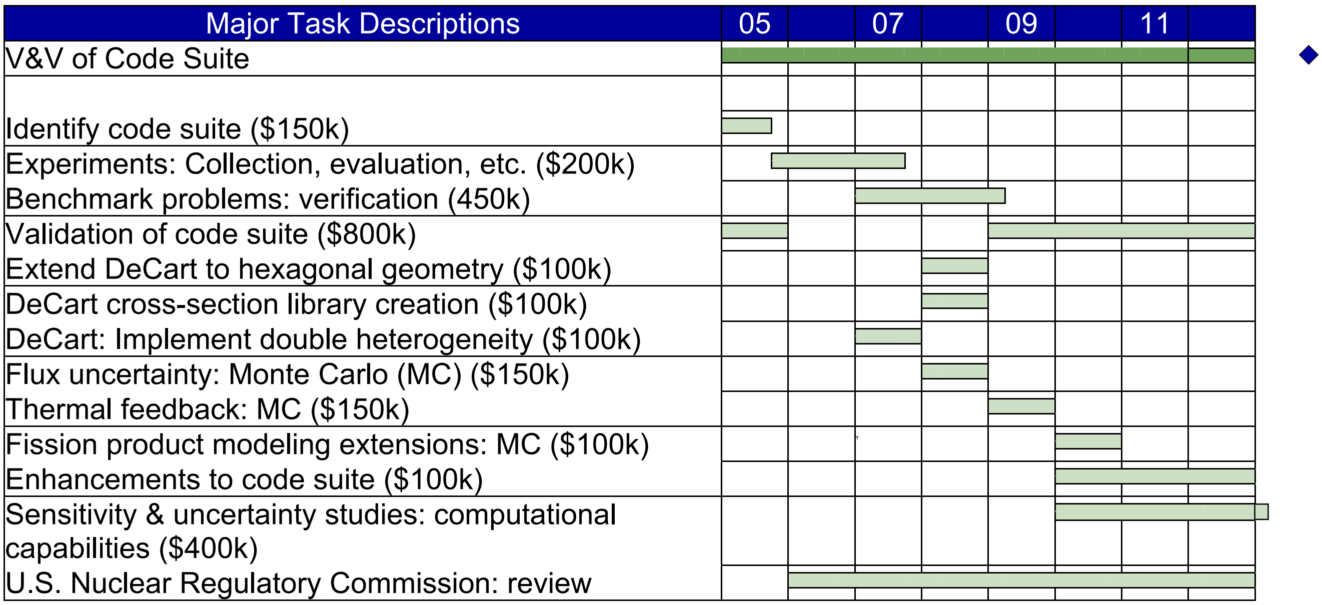


Figure 23. Timeline for verification and validation of code suite.

6. THERMAL-HYDRAULICS

The thermal hydraulics of the NGNP encompasses the heat generation by the fuel, its transport to the helium coolant, the laminar or turbulent flow of the helium as it flows from the upper plenum through the core, into the lower plenum, then out the exit duct to the secondary vessel containing the IHX or gas turbine that will extract the thermal energy from the helium. Also included are the heat losses from the reactor vessel during normal operation as well as accident scenarios that may occur due to failures in the system. Systems that are designed to remove the heat in the event of an accident, the reactor cavity cooling system, are also included in the thermal hydraulics of the NGNP.

Clearly, there is significant advantage to study the expected operation of the NGNP by using advanced simulation and analysis tools, backed by needed experimental validation data before actually building a prototype of the NGNP. Hopefully, simulation tools will help determine the possibility of achieving desired operating capacities, weed out less optimal designs, and prepare for possible accident scenarios to help ensure the safe and efficient operation and shutdown of the plant.

The flow and heat transfer in the NGNP are characterized by complex physics in complex geometries. Advanced simulation tools are available to simulate turbulent flow and heat transfer in engineered systems. It is desired to validate such tools to determine their usefulness for applications to the NGNP. It is fully expected that advanced computational fluid dynamics (CFD) codes will be needed to simulate regions of complex turbulent flow in the plant. Because of the size and complexity of the plant, it is currently expected that thermal hydraulic systems analysis codes can be applied, perhaps in conjunction with CFD codes to fully analyze the plant. While CFD codes can simulate flow and heat transfer physics using first principles, systems analysis codes rely on empirical data to represent key aspects of the thermal hydraulics such as wall heat transfer coefficients and friction factors. However, most CFD codes rely on some form of turbulence model to represent turbulent flow physics. Of course, neutronics/fluid behavior interaction will also be important to analyze the NGNP.

While it is clearly desirable to attempt to validate existing CFD and systems analysis tools, it may eventually be necessary to develop more advanced numerical simulation tools to handle the tremendous complexity and size of the NGNP. It is believed that a multi-track approach should be pursued for the thermal hydraulics aspects of the NGNP analysis, including (1) validate existing available tools, (2) develop existing tools as necessary and (3) pursue R&D to obtain more efficient and effective simulation tools that may take several years to develop. Track 3 is a parallel track that will help ensure that needed simulation tools will be available in the future that may be even more efficient than existing codes.

The near term thermal hydraulic tasks follow the first track above, validating existing tools. As the simulation tools are tested for validation, it may become necessary to add new turbulence models or pursue other modeling strategies, such as large eddy simulation (LES), thus following Track 2. Tasks that follow Track 3, developing new methods, will be addressed as funding is made available (see Section 6.2). The commercial CFD code Fluent and the systems analysis code RELAP5-3D will initially be validated and developed for the near term thermal hydraulics tasks.

6.1 Methodology Used to Define Thermal-Hydraulic R&D

The methodology applied to ensure the thermal-hydraulic software can be used with confidence to calculate the behavior of the VHTR is outlined and discussed in Section 3. However it is useful to outline how the methodology will be specifically applied for the R&D outlined in this chapter.

The R&D process will progress as follows:

a. **The R&D is based on the latest PIRT.** Presently the only available PIRT is the "first-cut" PIRT outlined in Section 3.2. However, as the design of the VHTR matures a successively more sophisticated PIRT will be required to identify the key scenarios and important phenomena (see Figure 24—step i). Hence the R&D plan is based on the assumption that an ever-improving PIRT will be available. Thus it is clear that all phenomena that must be calculated have not yet been identified. A formal PIRT should be created in conjunction with the pre-conceptual design in approximately 2006 or 2007 and then updated as the conceptual design, the preliminary design, and finally the final designs are formulated.

b. **The software used to analyze the VHTR behavior must be validated for the scenarios of importance.** The process thus begins using existing data. If either existing data are not available or the existing data are not adequate to cover the VHTR's operational envelope, then experiments must be defined, built, and data produced to provide the basis for software validation (see Figure 24—steps ii and iii).

c. **If the validation studies show the software cannot adequately calculate the key phenomena in the important plant scenarios, then development must be done to improve the software or alternatively more sophisticated software must be used if available or developed if not available (Figure 24—steps iv and v).**

d. **Once the software has been validated and shown to be capable of calculating the important phenomena to the accuracy needed (Figure 24—step vi), then best-estimate analysis may begin.**

6.2 Thermal-Hydraulic Software

Thermal-hydraulic software falls into three categories: (i) systems analysis, (ii) computational fluid dynamics (CFD), and (iii) severe accident. Systems analysis and CFD codes are shown in Figure 8 and each will be discussed briefly:

Systems Analysis. Systems analysis codes, such as RELAP5-3D© and GRSAC were originally designed to obtain one-dimensional calculations of an entire system such as an advanced gas-cooled reactor—including the balance-of-plant if necessary. While such codes may have the capability to model multi-dimensional effects, their capacity to produce widely accepted analyses of multi-dimensional behavior is limited by the assumptions and capabilities that stem from their field equation formulations. The field equations are usually first-order approximations. Characteristics of systems analysis code models are: (a) the calculations generally converge rapidly and thus don't require extensive computer resources, (b) the nodalizations are relatively coarse, i.e., a few hundred cells, (c) the models are constructed cell-by-cell by the analyst, and (d) the calculations provide ideal boundary conditions for other software such as CFD.

The predominant systems analysis software has extensive V&V matrices, a large user community, and are commonly used in the nuclear industry.

CFD: The CFD world is large and rapidly increasing in size. Common commercial CFD codes are Fluent, STAR-CD, and CFX. A number of famous CFD codes have been produced by the national laboratories—such as SOLA, CFDLib, Telluride, etc. The field equations, although often represented by first-order approximations, are generally represented by second-order approximations for best-estimate calculations. Characteristics of CFD models are: (a) the calculations may converge slowly and may

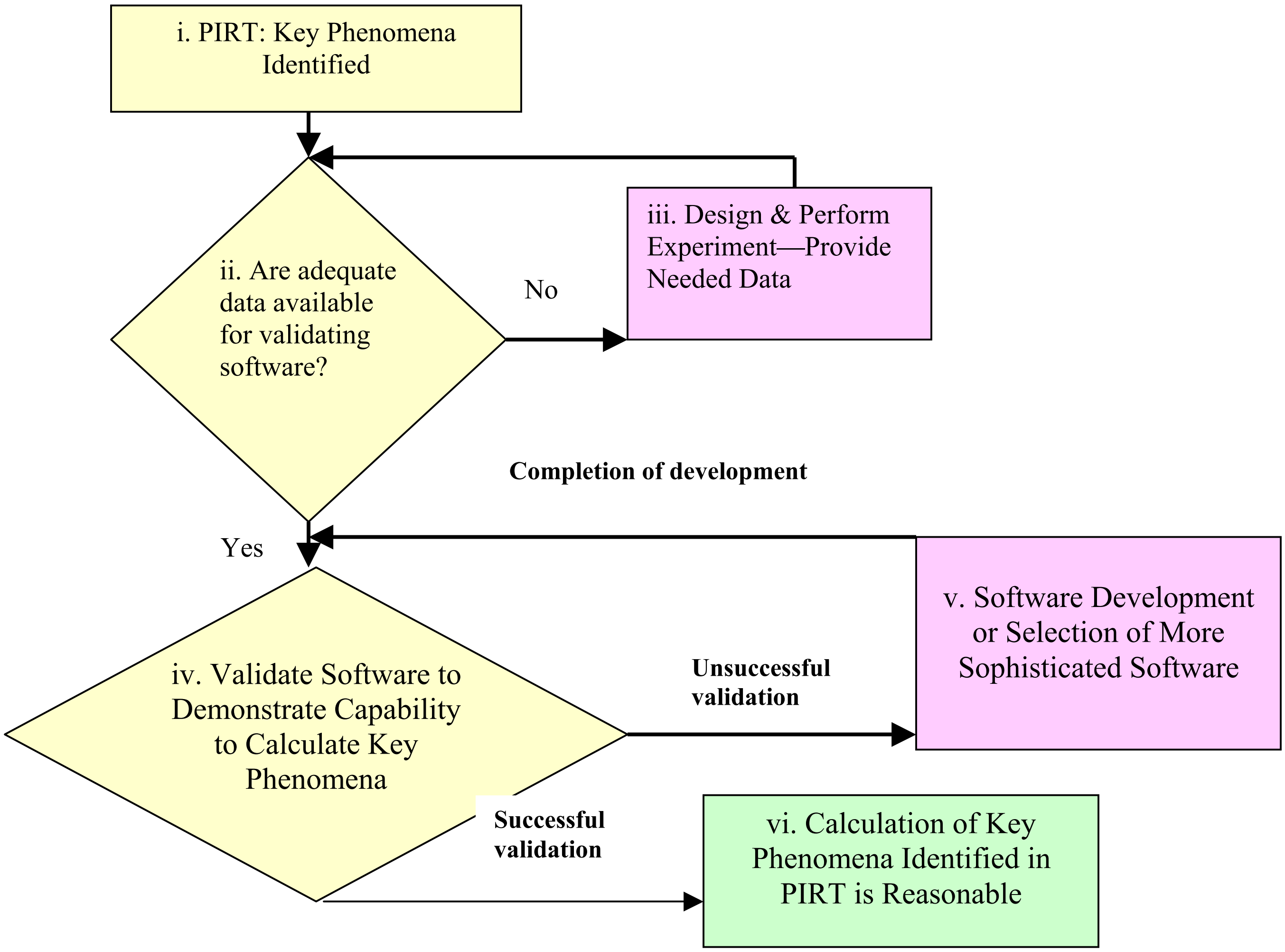


Figure 24. Methodology used to define thermal-hydraulic R&D.

require state-of-the art computing requirements to obtain a solution in a reasonable time, (b) the nodalizations may have many thousands of computational cells, hundreds of thousands, or even millions of cells dependent on the region that requires analysis, and (c) the models are generally produced using other software called mesh generators.

Regarding the CFD software, the large commercial CFD software have large user communities, large V&V matrices, and are generally user-friendly. The more well known CFD software produced by the national laboratories generally have a much smaller user community (in relation to the commercial CFD codes), smaller V&V matrices that are sometimes focused on particular problem classes, and are generally not user-friendly. The extreme case for CFD codes are those developed by individual developers to examine specific problems.

Another characteristic of CFD modeling is the approach taken for calculating the influence of turbulence, for example to estimate the degree of mixing that occurs in a plenum. One of the more common approaches is accomplished by taking an average of the incompressible Navier-Stokes equation to obtain the Reynolds-Averaged Navier-Stokes equations (RANS) as described in Speziale & So, 1998. A newer approach toward predicting the ensemble average of the fluid velocity is called large eddy simulation (LES) "…in which the Navier-Stokes equation is 'filtered' instead of averaged. This generates equations for the large flow scales yet uses a 'subgrid' model to capture the effect of the smaller scales." (Bernard et al. 1998, p. 13-3) Finally, the direct numerical simulation (DNS) approach of representing the Navier-Stokes equations enable all turbulence scales to be resolved.

RANS, LES, and DNS all may become ingredients in the R&D effort depending on the calculational requirements for the NGNP scenarios. The CFD V&V and calculational efforts will begin by using a RANS approach, as available in commercial CFD codes such as Fluent, to model the turbulence in the VHTR component regions such as the lower plenum at operational conditions. If this approach proves to be inadequate, then several approaches to obtaining a more representative model are available. For example, the commercial CFD firms may release their source code for modification by the NGNP team. Or alternatively, CFD codes developed at the DOE national laboratories may be used. Inherent in this approach is the possibility of using at least a LES approach in addition to RANS. Finally, since the R&D effort will last in excess of six years, if both RANS and LES approaches prove to be inadequate, a DNS approach may be applied in specific cases. The R&D approach that will be followed, specific to CFD codes, is illustrated in Figure 25. In every case where multi-dimensional CFD calculations are required, e.g., to model turbulence, the process will begin by performing the required validation calculation using a well-known commercial CFD code (Step 1). If the validation proves to be inadequate with no hope of improvement, then either Track 2a, Track 2b, or Track 3 will be followed where Track 2a represents modifying the source code of a commercial CFD code (obtained in a partnership agreement with the commercial firm such as Fluent), Track 2b represents modifying the source code of an experimental CFD code such as CFDLib[e], and Track 3 is the creation of a CFD code as part of the Generation IV project specifically to address the problem of concern. At any time, as necessary, the CFD approach may move from a RANS approximation to LES. The use of DNS is low probability.

Coupled Systems Analysis & CFD Codes. Due to the almost opposite characteristics of systems analysis codes and CFD codes, e.g., coarse 1-D nodalization vs. fine 3-D nodalization respectively, these two types of software naturally lend themselves to coupling. Such an approach enables detailed, three-dimensional analyses to be performed using the CFD code (such as Fluent) while the boundary conditions required by the Fluent calculation are provided by the balance-of-system model created using the systems analysis code, such as RELAP5-3D©.

Presently Fluent and RELAP5-3D© are coupled using a technique that permits implicit interactions between them using an Executive Program. Hence, if necessary, the Executive will allow Fluent and RELAP5-3D© to move forward in calculation space on a time-step-by-time step basis. This approach is illustrated in Figure 26.

Presently the Fluent CFD code and the RELAP5 systems analysis code are implicitly coupled. Additional coupling options will be required to enable the full advantage to be utilized from this approach, e.g., (i) multiple sessions of CFD to systems analysis coupling (to permit two or more CFD models to be linked to

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e. CFDLib is the Los Alamos Computational Fluid Dynamics Library. This is a collection of codes. The CFDLib collection is a repository for the numerical methodologies that were developed in the Fluid Dynamics Group (T3), of LANL's Theoretical Division. For example the MAC method (due to Harlow & Welch); the ALE method (Hirt, et al); the multifluid ICE method (Harlow & Amsden); the FLIP method (Brackbill & Ruppel) are all schemes that reside in the CFDLib collection. In recent years the CFDLib collection has been made into a sort-of 'open-source' project, with contributors from all over the Academic world, as well as many other divisions of LANL and other US National Laboratories. For multiphase flow the original capabilities of K-FIX (Rivard & Torrey) are contained in CFDLib (see Kashiwa et al. 1993, 1994).

the systems analysis code[f], (ii) explicit coupling to permit heat transfer coupling to fluid boundaries, and (iii) neutronics coupling such that the RELAP5 neutronics package can be coupled to the CFD code.

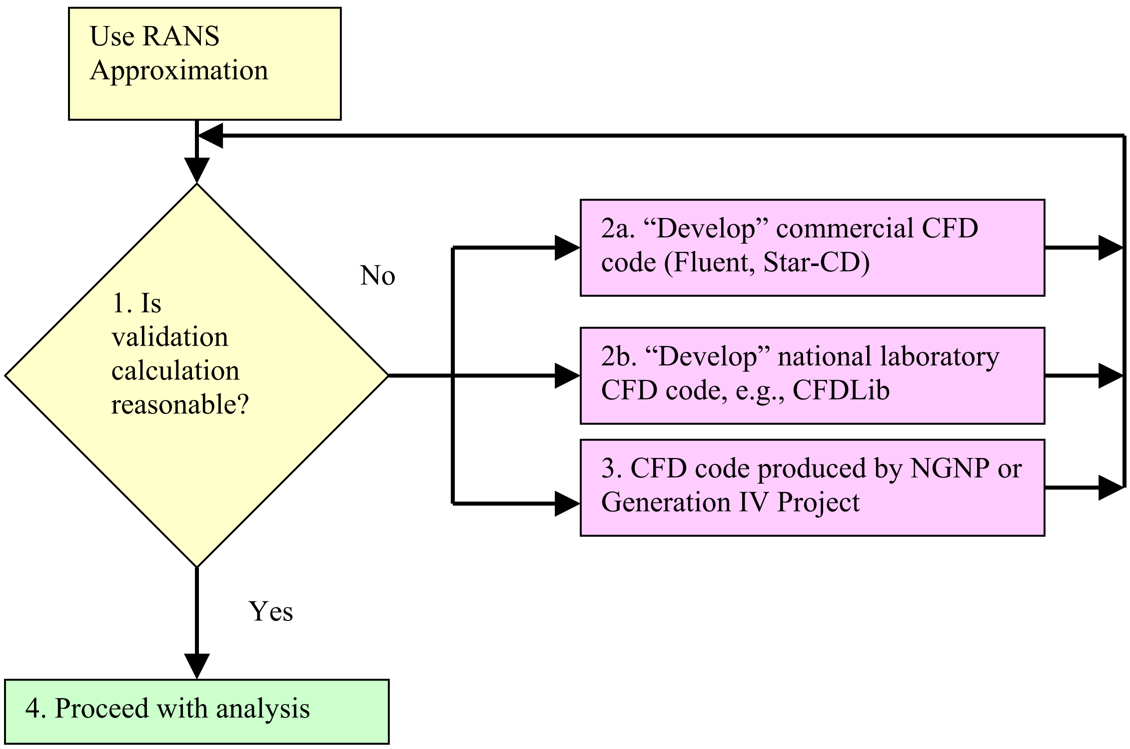

Figure 25. Approach for achieving validation objective for CFD.

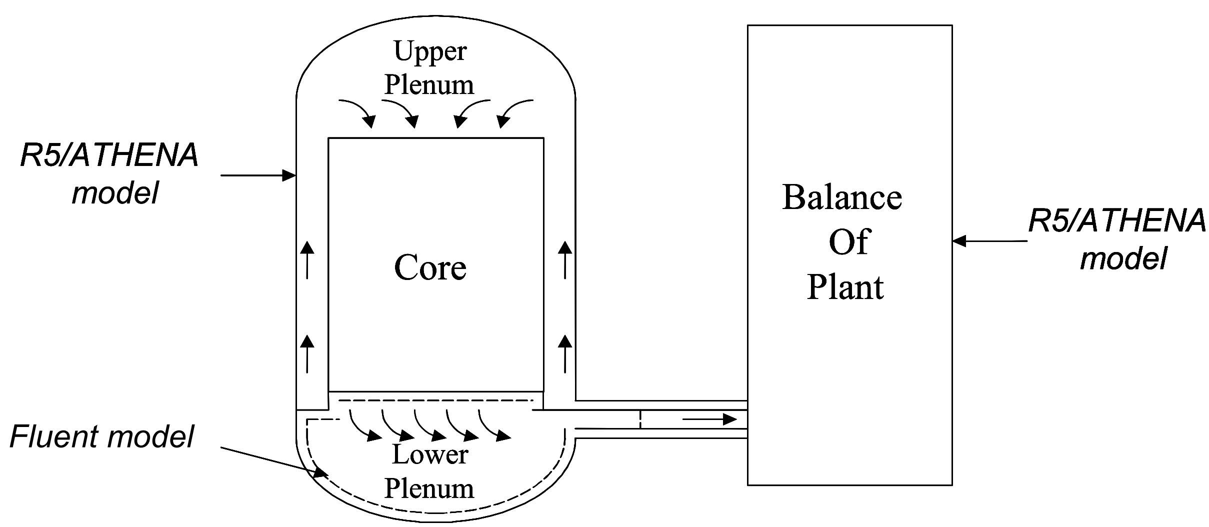

Figure 26. Illustration of coupled CFD and systems analysis code.

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f. When several CFD sessions may be linked to a systems analysis code then independent CFD calculations of various plena, such as the upper and lower plena, may be linked to the systems analysis model of the reactor.

6.3 Thermal-Hydraulics R&D Step i—the PIRT

The objective of defining a PIRT is to reduce all potential uncertainties to a manageable set to reduce the number of calculations, experiments, and validations to a manageable size (see Boyack 1990). The physical processes are first identified during a phenomena identification and ranking process (together with relevant plant components) and then ranked to establish process identification and ranking tables (PIRT) appropriate to the particular scenario and plant design. The identification and ranking should be justified and documented. The rationale is that plant behavior is not equally influenced by all processes and phenomena that occur during normal operation or a transient. The effort reduces all candidate parameters to a manageable set by identifying and ranking the phenomena with respect to their influence on the plant performance criteria or the primary safety criteria.

Since the NGNP design effort will probably have four phases: pre-conceptual, conceptual, preliminary, and final, the most useful approach from an R&D perspective, is to define the first PIRT during the pre-conceptual design stage. Thereafter, the PIRT could be easily updated during the three subsequent stages.

The PIRT should be defined by a group of gas-cooled reactor experts convened specifically for this purpose. The estimated cost of this activity is $50K for the pre-conceptual design. Updates to the PIRT to consider the changes embodied in the conceptual, preliminary, and final designs are estimated to cost $40K, $50K, and $100K, respectively.

6.4 Thermal-Hydraulics R&D Steps ii, iii, & iv—Experiments & Validation

It is known that some experiments are already needed (Step ii—see Figure 24)—since adequate data are not available that describe key phenomena identified in the "first-cut" PIRT. The quality of available validation data is discussed in Schultz, Ball, and King (2004. This section describes experimental programs that are needed (Step iii) together with their respective validation efforts (Step iv).

In keeping with the R&D process described earlier, the PIRT is initially used to identify the key phenomena that are expected to be present during NGNP operation. Once these phenomena are identified, the system analysis (RELAP5-3D/ATHENA or GRSAC) and CFD (Fluent, STAR-CD) tools are initially validated against existing experimental data. The results of this process will indicate where additional data are needed, for both model development and further assessment. It should be noted that the detailed scope of planned experiments has a large uncertainty in the out-years. However, it is felt that experiment work in the general categories described below will still be needed.

6.4.1 Matched Index of Refraction (MIR) Lower Plenum Experiments & Validation

The unheated MIR experiments are the first steps to analyze fluid behavior in a complicated geometry configuration such as the lower plenum. A photograph of the MIR facility at the INEEL is shown in Figure 27. The MIR experiment will simulate flow features of the paths of hot jets as they mix while flowing through the array of posts in a lower plenum en route to the single exit duct, as shown in the sketch on the right hand side of Figure 27. Useful optical flow measurements in this realistic configuration would be impractical without refractive-index-matching. Pointwise velocities and turbulence components will be determined in three directions by use of a laser Doppler velocimeter (LDV) system. A particle tracking velocimetry (PTV) system will be employed to measure the mixing of particles (representing thermal mixing) from the various jets emanating from simulated reactor cooling channels. Simulated plenum dimensions will be based on geometrical scaling of a current NGNP concept.

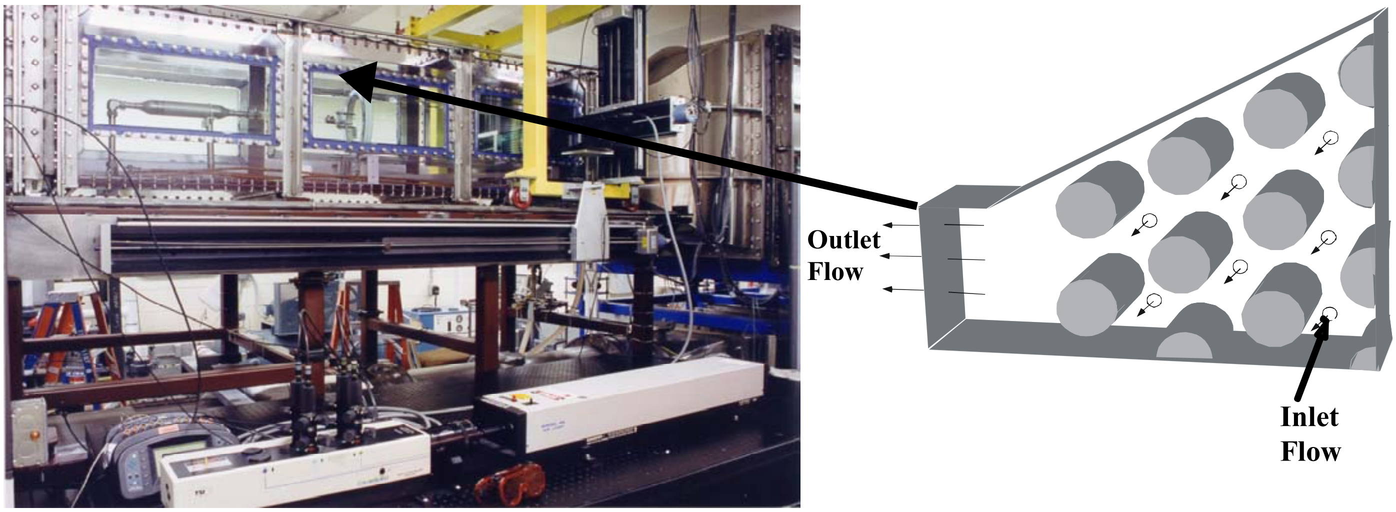

Figure 27. Mixed index of refraction facility (left) and preliminary mock-up of test section (right).

The extent of the mixing of the flow exiting the core as it migrates to the exit duct will determine the maximum temperatures that will be experienced in the lower plenum, the exit duct, and by the IHX or the turbine.

The flow enters the lower plenum from scores of coolant channels as downward moving jets. The flow then turns 90 degrees as it heads for the outlet duct, while having to negotiate the cylindrical bars supporting the core. It is desired that the helium be well mixed in the lower plenum to minimize the temperatures seen by the materials in the lower plenum, the exit duct, and the IHX or the turbine. There are materials issues for each of these components as well as performance issues for the IHX or turbine for which the desired inlet conditions are a nearly uniform temperature. The turbulent flow in the lower plenum will be modeled using a CFD code to try and capture the complex turbulence and mixing effects. However, the turbulence model employed in the simulation effort must be validated as to its ability to model the complex physics of turbulent jets mixing in a crossflow that flows around a number of cylindrical supports on its way to the exit duct. This activity involves the validation of turbulent flow modeling strategies as well as the provision of validation data. The data will be provided by a scaled test section; the scaling laws will need to be developed in order to properly employ the validation data.

Scaling studies have begun in fiscal year 2004 to identify the relationships that relate the mean velocities U_i, Reynolds stresses $\rho u_i u_j$, the mean temperature T, and turbulent heat fluxes $u_i t$ between a scaled facility and the baseline VHTR. A first mock-up of the test section is shown in Figure 28 undergoing a visualization experiment.

The scaling studies will be performed to non-dimensionalize the relevant parameters and governing equations. With the equations written in terms of dimensionless groups the assumptions will be cast and the conditions documented under which equal dimensionless numbers in the scaled experiment and the full-scale reactor system represent equivalent conditions. An example of this is given in a predecessor to the ongoing scaling study (Cochran et al. 2004):

$$\frac{Gr_{\Delta T}}{\mathrm{Re}^2} T^* - \frac{\partial \tilde{p}^*}{\partial z^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} \left[\left[\frac{1}{\mathrm{Re}} + \frac{\mu_t}{\rho VD} \right] r^* \frac{\partial u^*}{\partial r^*} \right] = 0 \quad (1)$$

for a passive condition where Gr = Grashof number, Re = Reynolds number, and p^*, z^*, r^*, u^*, and T^* are the dimensionless pressure, z-coordinate, r-coordinate, velocity, and temperature for the system.

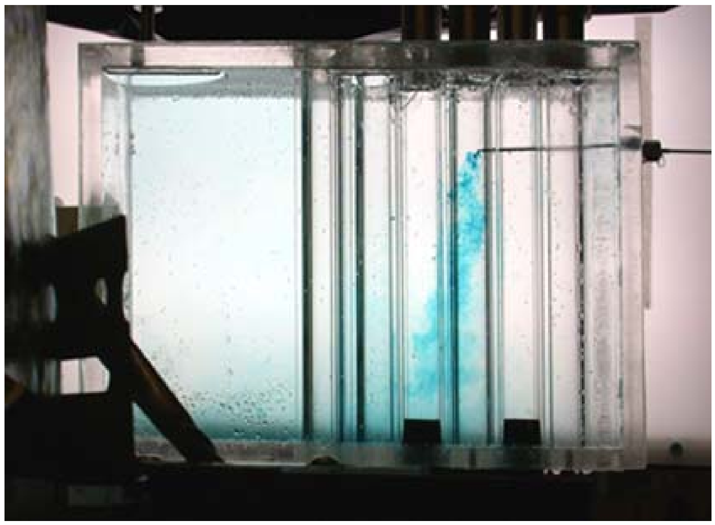

Figure 28. A visualization experiment to study lower plenum mixing.

The data provided by the MIR experiments will be used to validate the Fluent CFD code's capability to predict the turbulent mixing in the lower plenum of the reactor at rated operational conditions. The standard procedure that will be followed consists of performing: (i) a series of calculations during the experiment design phase to assist in finalizing the experimental test section, (ii) a blind calculation prior to each experiment to establish a benchmark, (iii) a comparison between the blind calculation and the measured data, and (iv) an evaluation of the capability of the CFD code to both match the data and model the key phenomena. Ultimately, from these calculations will come a measure of the predicted turbulence, an idea of where the active turbulence will be observed, and a benchmark to locate and specify the experimental instrumentation.

The item (i) calculations will also include a calculation of the behavior in the reactor lower plenum design itself. Having calculations of the mixing in the full-scale lower plenum and the experimental test section mockup of the lower plenum enables direct comparisons of the two and evaluations of the predicted turbulence and mixing. A preliminary calculation of the mixing the GT-MHR lower plenum is shown in Figure 3.

Heated Experiments: Because the MIR is an isothermal experiment, performed at room temperature, heated experiments will be considered to address the influence of large temperature gradients in the lower plenum and their effect on mixing. Also to be considered are heated experiments aimed at evaluating the "hot channel" problem. Such experiments will provide documented temperature, velocity and turbulence fields for mixed convection (buoyancy effects) and gas property variation in NGNP cooling channels in order to assess codes and their turbulence models at reactor conditions for which benchmark data are not available. Instrumentation will include miniaturized multi-sensor hot-wire probes developed as a task in a recent INEEL NERI project for gas-cooled reactors.

The experimental databases, in part acquired in the heated experiments described in the above paragraph, will be used to validate Fluent's (or other CFD codes) capability to calculate best-estimate conditions and behavior in the VHTR "hot channel." This work will be combined with validation efforts based on measurements obtained through ongoing projects at Penn State and M.I.T.

6.4.2 HTTR and HTR-10 Experiments

HTTR Experiments: The Japan Atomic Energy Research Institute's (JAERI's) plans to perform a spectrum of experiments in their HTTR which are of great interest to the NGNP program. Among the experiments may be a LOCA, a pressurized conduction cooldown experiment, a rod ejection experiment, and an anticipated transient without scram. The HTTR became operational in 1998. The reactor vessel is 13.2 m tall (inner dimension) and has a 5.5-m inner diameter. The core has 30 fuel columns and 7 control rod guide columns. There are 12 replaceable reflector columns and 9 control rod guide columns. The HTTR is fitted with a RCCS system. The HTTR operates at 4 MPa with a core inlet temperature of 395 °C and outlet temperature of up to 950 °C. However, it is known that the HTTR does not have a full set of instrumentation. Thus to obtain the quantity and quality of data needed for tool development validation, additional instrumentation is required. The scope of work proposed for the HRRT experimental task would be for the NGNP Program to obtain access to the HTTR data through a collaborative agreement with JAERI. Potentially, the NGNP program could provide HTTR needed instrumentation, test planning, and analysis as was done for previous collaborative programs with JAERI.

HTR-10: The HTR-10 is a 10-MW pebble bed high temperature gas-cooled reactor that became operational in 2000. This reactor holds great promise for being a test bed that will provide data that can be used for thermal-hydraulic software validation. The HTR-10 reactor vessel (see Figure 11) is approximately 11.2 m in height and contains a 1.8 m diameter core that is 1.97 m high with ~27000 pebbles. The reactor was designed to operate at 10 MWt. The average power density is 2 MW/m^3 and the core inlet temperature is 250 to 300°C. The core outlet temperature will range from 700 to 900°C. However, no data are available to the NGNP Program since there currently are no collaborative agreements between the USDOE and INET. However, HTR-10 has been providing benchmark data to the international community. Presently there is an international problem exercise ongoing via the International Atomic Energy Agency (IAEA) based on a loss of primary flow without scram and a control rod withdrawal without scram. The actual workscope for this task will be to help facilitate an agreement that will make the HTR-10 data available to the NGNP Program and to develop a detailed workscope for tool development and assessment. The quality level of the HTR-10 data is unknown. However, it is believed the data are high quality. Another unknown is the quantity of measurements and types of measurements available. This issue will have to be considered in developing a collaborative agreement with INET.

Validation Studies Based on the HTTR and HTR-10 Experiments. Design experiments relevant to the performance and behavior of the VHTR will be performed in the HTTR and HTR-10 during the next few years. We plan to participate in that work. In particular, we will define the quantity, range, and placement of extensive instrumentation for both facilities and perform blind calculations for each experiment for which the United States will receive data. Following each experiment, we will perform a data evaluation and a counterpart calculation using both RELAP5 and Fluent. Finally, we will perform parametric calculations to examine factors that will influence the behavior of the experiment such that the most demanding conditions could be experienced. Approximately two experiments should be examined per year in each facility.

6.4.3 Scaled Vessel Experiment

Code development and assessment activities for previous reactor designs have required integral type experiments at different scales to verify that small scale laboratory experiments, experiments using simulated fluids, and experiments at non-rated conditions have been properly scaled to the full scale plant. This premise holds true for any NGNP design. While some large-scale integral test data will become available from HTTR and HTR-10, there will undoubtedly be a data gap when considering the phenomena resolution needed to validate linked systems codes and CFD calculations. To help eliminate distortions caused by data gathered in small-scale facilities, a large scaled vessel experiment will be performed. A highly instrumented, geometrically correct, large-scale vessel simulator will be constructed consisting of a upper plenum, core simulator, lower plenum, hot duct, and the turbine inlet channel. Geometry will be dictated by the best available information available as to the details of the actual design configuration. The actual scale of the facility required will be determined from previous experimental results and available literature, as well as the phenomena expected to be present as determined from available design information. Facility size on the order of 1/4 to 1/3 scale is envisioned with subscale pressure and temperatures. The core simulator will be electrically heated and overall instrumentation will be sufficient to provide detailed local data for comparison to CFD codes as well as global data for system code comparisons and assessment. The facility will be capable of simulating both operational conditions and accident scenarios. Issues that can be studied for operational conditions include the influence of various bypass conditions on the system operational envelope, the progression of mixing and turbulence of the helium as it moves from the lower plenum through the hot duct to the turbine inlet, and the influence of various lower plenum configurations on the system performance. Accident conditions that can be examined include the influence of natural circulation on the thermal behavior of the system during the depressurized conduction cooldown scenario among others.

Using the experimental data obtained in the large scaled vessel experiment, a set of comprehensive code validation activities will be performed. The standard procedure that will be followed consists of performing: (i) a series of calculations during the experiment design phase to assist in finalizing the experimental test section, (ii) a blind calculation prior to each experiment to establish a benchmark, (iii) a comparison between the blind calculation and the measured data, and (iv) an evaluation of the capability of the CFD code and systems analysis code to both match the data and model the key phenomena. The fluid behavior, as it moves from the lower plenum to the upper plenum through the core will be analyzed using the Fluent CFD code coupled to RELAP5-3D. Fluent will be used to predict the mixing behavior in the plena whilst RELAP5-3D will be used to model the balance-of-the-system.

6.4.4 INEEL Mixed Convection Experiments

As part of an INEEL Laboratory Directed Research and Development project, MIT and INEEL developed an experimental facility (see Figure 29 and Table 7) to study mixed convection heat transfer regimes shown in Figure 6. Once the LDRD work is completed in 2006, the equipment will be transferred to the INEEL. Further experiments are planned in the facility at the INEEL. In addition to expanding the data set obtained by MIT, additional INEEL experiments should be performed to satisfy the data needs identified by the PIRT and assessment studies.

The validation effort, based on the above experimental facility, will be aimed at both correlation development and validation for systems analysis codes and validation of CFD codes. For the development/validation effort centered on systems analysis codes, the objective will be to demonstrate the correlations are applicable to the flow region between laminar and turbulent flow. CFD calculations will be performed (experiment design, blind pre-experiment, and post-experiment analysis) to study the calculated velocity profiles and heat transfer coefficient behavior in the facility.

6.4.5 Argonne National Laboratory Reactor Cavity Cooling System Experiments

The objective of this task is to acquire the model/code validation data for the natural convection and radiation heat transfer in the reactor cavity and the reactor cavity cooling system through performance of experiments in the ANL Natural Convection Shutdown Heat Removal Test Facility (NSTF) shown in Figure 30.

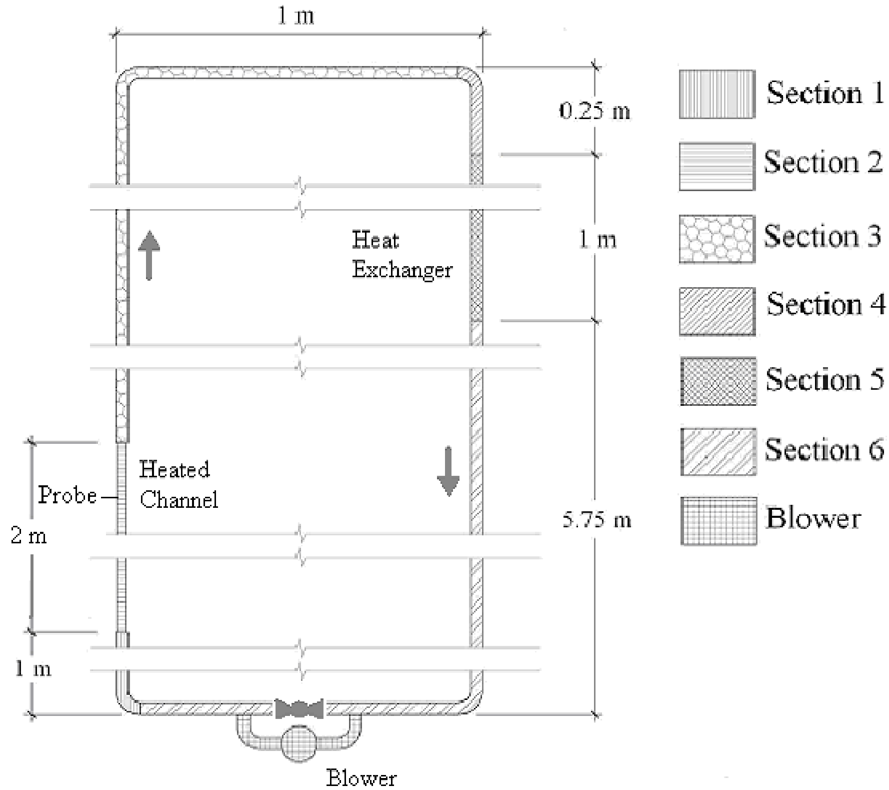

Figure 29. Mixed convection heat transfer correlation development facility.

Table 7. Component description of mixed convection loop.

Section	Description	Diameter	Material	Roughness	Height	Length	Form Loss[a]
1	Upcomer	25.4 mm	SS 316	1E-5 m	1.00 m	1.00 m	0.50
2	Heated CH.	16,32 mm	SS 316	1E-5 m	2.00 m	2.00 m	0.68,0.40
3	Hot Leg	25.4 mm	SS 316	1E-5 m	4.00 m	5.00 m	0.50
4	Downcomer	25.4 mm	SS 316	1E-5 m	0.25 m	0.25 m	0.50
5	Heat Ex.	25.4 mm	SS 316	1E-5 m	1.00 m	2.00 m	0.00
6	Cold Leg	25.4 mm	SS 316	1E-5 m	5.75 m	6.75 m	0.50

a. Form losses based upon turbulent flow elbow bends and sudden expansion/contraction (Schmidt et al. 1993)

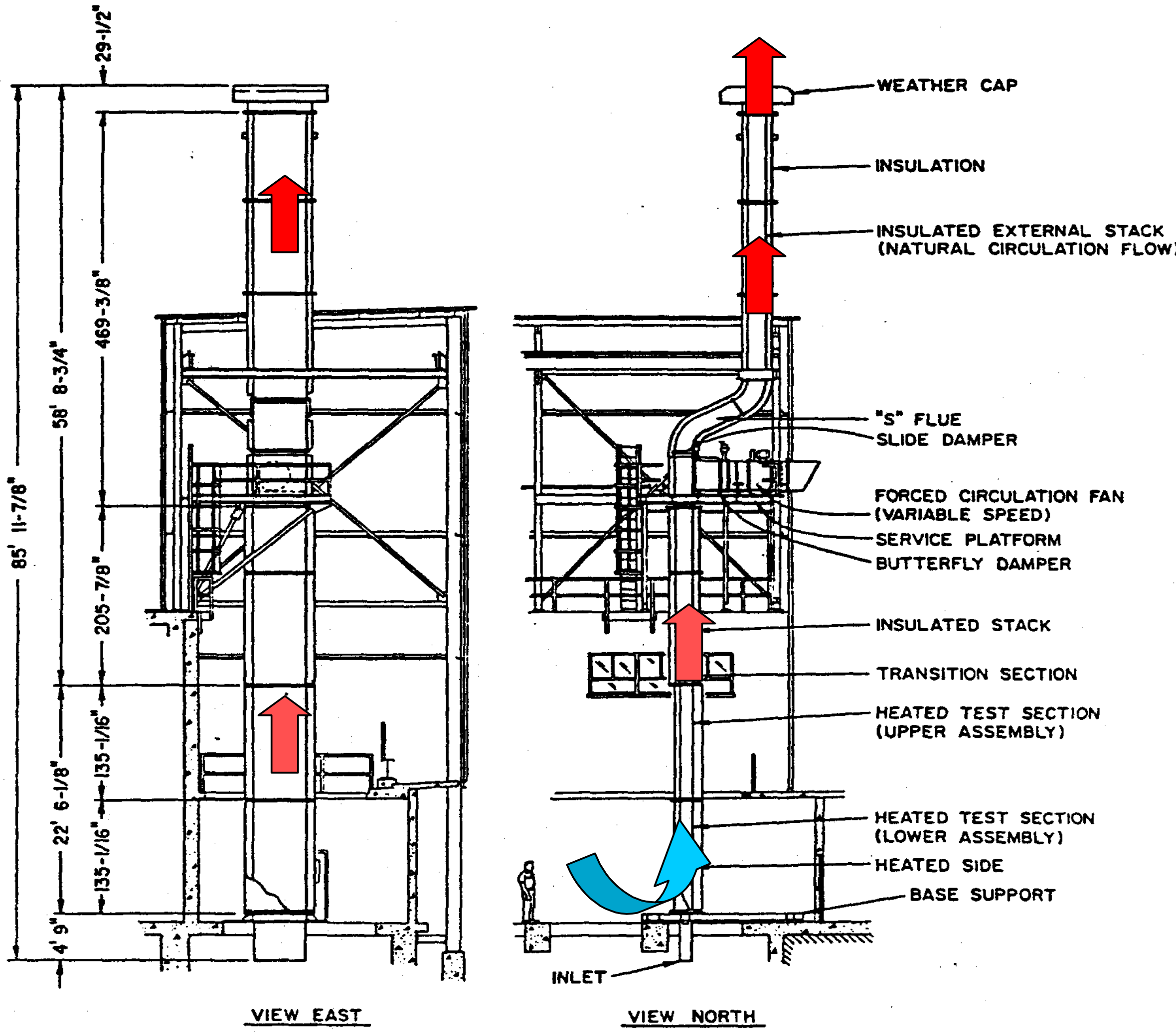

Figure 30. ANL reactor cavity cooling system test facility.

The NSTF will be used as an RCCS experiment "simulator". The first task will be to determine scalability of the existing data from the ANL RCCS simulator to the RCCS design and the feasibility of using the ANL RCCS facility for generating scaled RCCS data. The scaling studies will identify the important non-dimensional parameters for each separate effects study. Based upon the results of the scaling study, the range of experiment conditions will be determined as well as the appropriate experiment scale and appropriate fluids to be used that most effectively simulate full-scale system behavior. Also, the RCCS design candidates (both the pebble-bed and prismatic options) and the range of thermal-hydraulic conditions will be identified. The feasibility studies will determine if any potential reconfigurations, power requirements, and instrumentation modifications would be required. An instrumentation strategy to assure that adequately detailed velocity and turbulence profiles, as well as surface pressure and/or temperature distributions for the validation of multidimensional simulation tools will be developed. Based on the results of these feasibility studies, a detailed engineering modification plan for the ANL RCCS facility will be developed. The engineering modifications will be implemented, start-up approval obtained and facility start-up testing performed to ensure satisfaction of the experimental requirements. Next, a test matrix will be developed and the indicated test program performed. The ANL RCCS experimental results will capture key phenomena expected to be present in the RCCS as well as providing data of sufficient resolution for the development and assessment of applicable CFD (STAR-CD/Fluent) and system codes (RELAP5-3D/ATHENA).

The computer code validation effort will consist of development of the experimental matrix, performance of pre-experimental design calculations, performance of blind calculations, and post-calculational analysis. The experimental matrix will cover the NGNP normal operational conditions as well as the expected depressurized conduction cooldown and pressurized conduction cooldown accident conditions. For the selected candidate systems the RELAP5/ATHENA system models will be constructed and a range of accident scenarios will be studied to obtain the range of boundary conditions for overall global parameters. A set of either STAR CD or FLUENT models for the selected candidate RCCS systems will be defined and the corresponding CFD calculations for a selected set of driving boundary conditions within the range determined by the RELAP5/ATHENA results will be performed. These results and the results of the FY-05 scalability study will be used in the selection of the matrix and the derivation of experiment criteria. Empty cavity, single tube and multiple tube experiments will be considered in the matrix planning for baselines. Since the facility operates in one of two thermal modes (a) constant (uniform) wall temperature or (b) constant (uniform) heat flux, both will be used. The system also accommodates stepwise variation of either mode singly, or in combination—so this feature will be used as well in the definition of the experiments. A selection will be made based on the relevant decay heat levels, vessel wall temperatures and power profiles based on the RELAP5/ATHENA system results.

Using part of the experiment database information, 1-D models will be developed which can be implemented in the RELAP5/ATHENA system codes. The RELAP5/ATHENA models will be used to obtain measures to compare against other parts of the database. The results of the scalability study from FY-05 will be used to select the appropriate groups of nondimensional variables. Based on the RELAP5/ATHENA system calculations and STAR CD or FLUENT calculation of candidate RCCS systems utilized in the selection of the experiment matrix, the plant conditions will be classified into separate phenomenological ranges. STAR CD or FLUENT CFD calculations will be performed for experiment planning and the results acquired from the performance of the experiments will be used to determine the optimum form for the correlation fit. The data analyses required to produce the optimum correlation fits with the selected scaling variables for each category of range of conditions will be performed. ANL will work with the RELAP5/ATHENA code developers to implement any new models/correlations in the code. Appropriate validation data from the part of the database which was not utilized in the model/correlation development will be selected and the models/correlations will be tested against those experiments.

With respect to CFD code validation, reviews of the experiments, experiment plans and procedures will be completed and the experiments in the matrix will be performed. A STAR CD or FLUENT model will be constructed of the experiment configuration. Parametric studies will be performed to define the meshing. For experiments in the matrix, CFD calculations with the given boundary conditions will be performed. These results and the results of the FY-05 scalability study in the design and planning of the experiment will be used to aid in the location and selection of instrumentation. The geometry of the experiments, gap size, tube size, and spacing will be set. The results will be also analyzed to confirm that experiment goals and criteria can be achieved. Because of the large thermal time constant associated with the experimental facility, thermal transient analyses will be performed with models of the experiments to define experiment start-up procedures as part of the experiment planning. Data analysis techniques, filtering and experiment diagnostics will be applied to select the appropriate data for archival in the database. A database will be developed with automatic queries to aid in the utilization of the information in the code/model validation work.

The Star-CD or Fluent CFD codes will thus be validated against the experimental database for the prediction of RCCS performance under operational conditions, depressurized conduction cooldown and pressurized conduction cooldown. Appropriate meshing strategies, structures and length scales for RCCS modeling will be studied for each condition. Appropriate turbulence modeling strategies and numerical schemes for each condition will be identified and used.

6.4.6 Bypass Experiments

A series of experiments are visualized that will test the various theories regarding factors that influence the quantity of bypass (in either the prismatic or pebble-bed) as a function of various factors including manufacturing tolerances, core configuration changes due to irradiation or thermal expansion. These experiments may or may not be an ingredient of the large scaled vessel experiment discussed in Section 6.4.3.

6.4.7 System Performance Enhancement Features: Validation Experiments and Calculations

The candidate VHTR designs will be reviewed to identify potential local design features in the area of insulation, baffles, mixing plates and other mechanical structures envisioned to enhance mixing, reduce thermal gradients and stresses and mitigate other structural issues. A list of basic geometries that are representative of important local features that are likely to have a limiting effect on system performance will be developed.

Scaling studies will be performed to identify the important non-dimensional parameters for each separate effects study. Based upon the results of the scaling study, the range of experiment conditions to be considered will be identified, the experiment scale will be determined and the appropriate fluids to most effectively simulate full-scale system behavior will be selected. The previous ANL IFR mixing experiments with simulant fluids and other experimental databases will be used to identify data sets containing detailed velocity, turbulence, and/or temperature profiles that are suitable for multi-dimensional CFD validation. We will then evaluate the applicability of these data sets to the candidate designs based upon the results of the scaling studies. Based on the study of geometries and flow conditions, we will develop a matrix of laboratory-scale experiments that would be used for code validation and model development.

To design the experiments, we will develop an instrumentation strategy to assure that adequately detailed velocity and turbulence profiles, as well as surface pressure and/or temperature distributions for the validation of multidimensional simulation tools are captured. Complete preliminary CFD simulations of the proposed experiments will be performed to aid in the placement and operation of instrumentation. We will also develop a detailed experiment plan and complete all necessary reviews, assemble and test the experiment set-ups, carryout the experiments in the matrix and archive the flow and temperature measurements as a database for the validation of potential turbulence modeling strategies within multidimensional CFD codes.

Using the CFD Code Star-CCM (Complete Continuum Mechanics) complete a validation study of computational mesh generation and turbulence modeling strategies for the simulation of the completed experiments (e.g., see Figure 31). If fluid-structure interaction is an important phenomenon in the selected separate effects experiments, capabilities for fluid structure interaction modeling within the Star-CCM code may be utilized or the code may be coupled to a separate solid mechanics software package. If necessary, additional model development for the code will be carried out. The data and code can then be used in the design of larger scale integrated experiment facilities and confirmatory calculations.

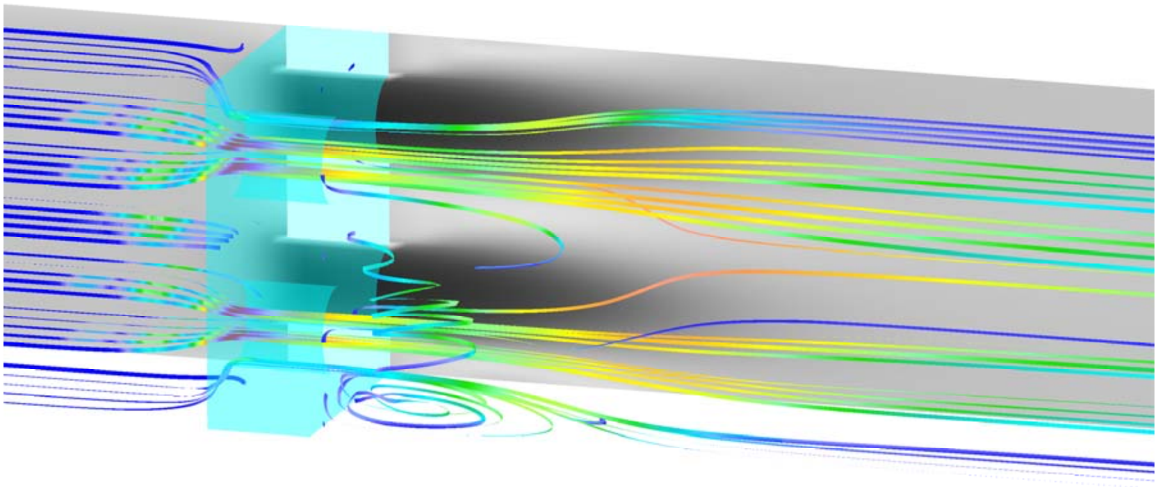

Figure 31. Predictions of fluid dynamic behavior within a rectangular duct in the vicinity of a 4-hole orifice plate (shown in cyan). Streamlines indicate motion of massless particles released into the fluid stream and are colored to show local turbulent viscosity. The grayscale cutting plane, which passes through the two rear orifices indicates local velocity magnitude.

6.4.8 Summary

The timelines for the planned experimental activities and the supporting validation efforts are shown in Figures 32 and 33. The total estimated costs for these efforts are $9,250k and $10,300k, respectively.

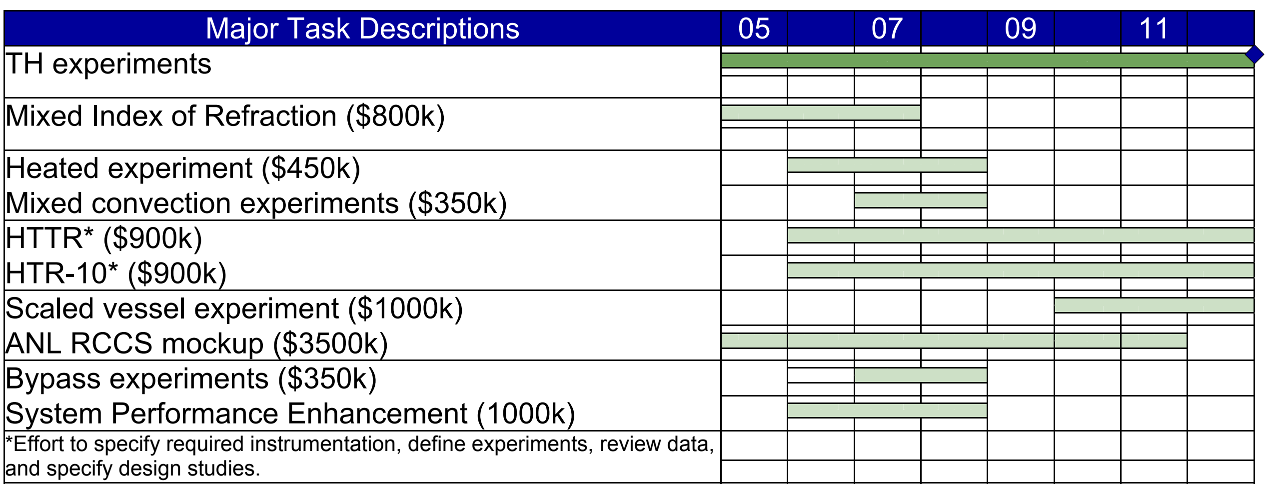

Figure 32. Timeline for thermal-hydraulic experimental R&D.

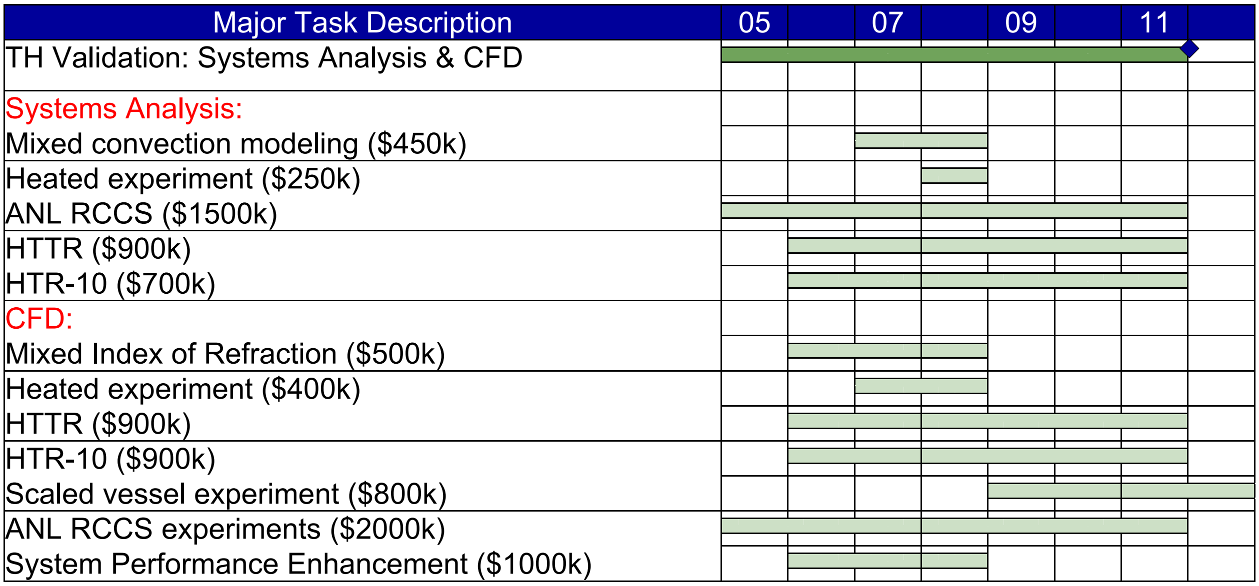

Figure 33. Timeline for thermal-hydraulic R&D new experiment validation: systems analysis and CFD.

6.5 Thermal-Hydraulics R&D Step iv—Validation

Some data sets are already available for validating systems analysis software and the CFD software and are identified by Schultz, Ball, and King (2004). Consequently, these validation activities can begin immediately and do not require additional experimental efforts.

6.5.1 AVR

Based on the drawings, specifications, and data obtained during the AVR project (acquired by DOE), build a model of the plant and perform a series of validation calculations that include the loss-of-coolant accident tested at AVR. Using the data acquired by inserted instrumented pebbles, during normal operation, perform neutronics calculations, using an appropriate systems analysis code, to study the calculated vs. measured pebble-temperature behavior. See Schultz, Ball, and King (2004) for further details.

6.5.2 Core Heat Transfer Modeling

The proposed R&D is aimed at breaking the problem down to its common denominator, i.e., a primitive that is represented by the triangle shown in Figure 34. Using the correct number of primitives a prismatic hexagonal block can be accurately represented. Thus the primitive forms the link between a RELAP5 material model that represents each block in the prismatic reactor and studies that may be done using finite elements codes that subdivide each block into a large number of mesh cells.

This activity focuses on RELAP5 systems code development aimed at modeling each prismatic block as well as performing calculations using software such as Fluent, Abaqus, etc. to obtain an in-depth temperature distribution of the hot blocks.

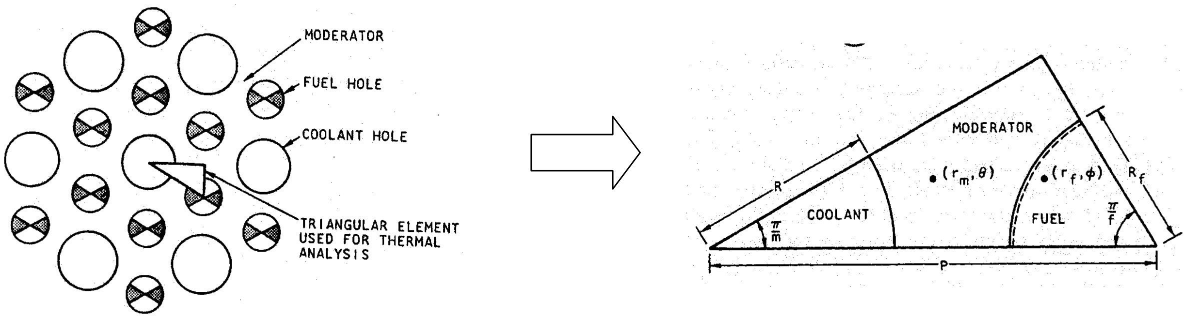

Figure 34. The primitive for a prismatic reactor.

6.5.3 HTTR RCCS Separate-Effects

Data were obtained in a series of 6 tests performed to simulate the heat transfer to the RCCS cooling panels (IAEA 2000). The experiments are summarized in Table 8. For these experiments cooling panels were placed inside a pressure vessel. Experiments were performed by varying the gas in the pressure vessel to change the natural convection characteristics; thus Experiment I was performed with a vacuum so no natural convection would occur and the only heat transfer from the heaters to the cooling panels would be radiation. Experiment III was performed with nitrogen and the remainder of the experiments were performed using helium. Also the cooling medium in the cooling panels was run with water for 4 experiments and air with 3 experiments. The power level was changed as shown.

The data summarized in Table 8 are ideal validation data for RELAP5 and also provide some useful validation basis for CFD calculations.

Table 8. RCCS experiments: HTTR Project.

Experiment	**I**	**II**	**III**	**IV**	**V**	**VIa**	**VIb**
Gas	vacuum	helium	nitrogen	helium	helium	helium	helium
Presssure (MPa)	1.3×10^{-6}	0.7	1.1	0.47	0.64	0.96	0.98
Power (kW)	13.1	28.8	93.9	77.5	29.7	2.6	8.0
Cooling panel	water	water	water	water	air	air	air

6.5.4 Sana Experiments

Sana was an experiment designed to study the heat transfer mechanisms and to provide the basis for validating the models required to determine whether sufficient energy can be transferred to the environment to prevent the fuel from becoming damaged following failure of all heat sinks with a simultaneous depressurization. As a part of the experiment, the measurement of the time dependent three-dimensional temperature distribution was completed and studied, the effective heat conductivity as a function of temperature was determined, and the heat fluxes were studied at the various reactor boundary sections. To make use of these data, we will build a model of Sana and perform calculations that can be used to validate RELAP5 and Fluent. The SANA experiments consist of a simulated pebble bed core filled with 9500 pebbles (diameter = 6 cm). The core simulator is cylindrical in geometry and has an diameter of 1.5 m and a height of 1 m. Heat is generated using four electrical resistance heating elements; a maximum power of 50 kW can be generated.

6.5.5 Balance-of-Plant Components

We will acquire data that are representative for turbines, compressors, reheaters, and the very efficient intermediate heat exchanger (IHX) planned for use in the NGNP. We will build models of these components and perform the necessary validation.

6.5.6 Jets & Cross-Flow Data

We will perform Fluent benchmark calculations based on the jet and cross-flow data described in some detail by Schultz, Ball, and King (2004). Using these data as a basis for validation for fundamental phenomena that are related to the mixing in the lower plenum at operational conditions, will demonstrate whether Fluent is capable of calculating the phenomena that are the fundamental components of the complex turbulence present in the lower plenum during operational conditions.

The general categories to be considered during this study include: (i) flow through tube bundles, (ii) a single jet in an unconfined crossflow, (iii) multiple parallel jets in a stagnant environment, (iv) multiple jets in an unconfined crossflow, (v) a single jet in a confined crossflow, and (vi) multiple jets in a confined crossflow.

6.5.7 NACOK Experiment

The NACOK[g] experiments were designed to model a representative section of the core undergoing the effects of air ingression through the connecting vessel between the reactor pressure vessel and a steam generator vessel (a German design). Consequently, the pipe breach opens the cross-section of the hot gas duct for entry of air flow, which moves into the core and then returns down through the cold gas ducts and leaves through the outer annulus of the coaxial duct. On the basis of the available drawings, a Fluent model will be constructed and validation calculations will be performed.

6.5.8 Summary of Step iv Validation Studies

The timeline for the validation studies is shown in Figure 35. The total estimated cost for these activities is $2,650k.

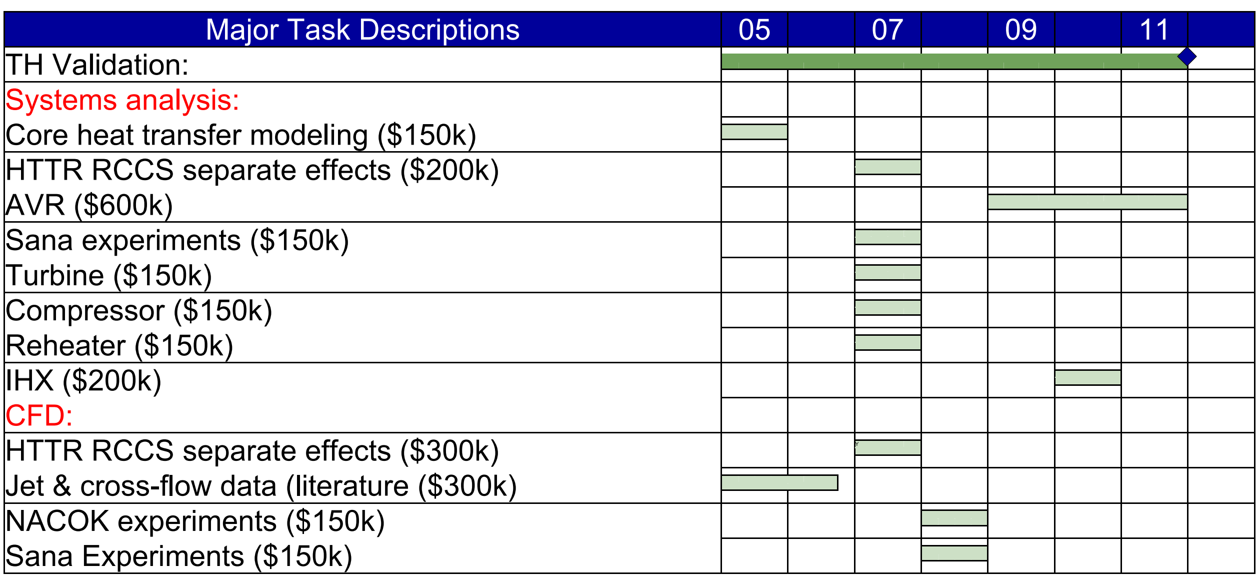

Figure 35. Timeline for thermal-hydraulic step iv validation effort.

g. NACOK = natural convection in the core with korrosion (corrosion).

6.6 Thermal-Hydraulics R&D Step v—Development

Development activities are centered in three broad areas: systems analysis, systems analysis and CFD coupled codes, and CFD.

6.6.1 Systems Analysis Code Development Activities

Systems analysis development activities include: core heat transfer modeling, mixed convection modeling, RCCS free convection modeling, multi-species modeling, an intermediate heat exchanger model, and diffusion modeling.

Core Heat Transfer Modeling. The development required to improve core heat transfer modeling in RELAP5, is centered on breaking the problem down to its common denominator, i.e., a primitive that is represented by the triangle shown in Figure 34. This activity focuses on RELAP5 systems code development aimed at modeling each prismatic block as well as performing calculations using software such as Fluent, Abaqus, etc to obtain an in-depth temperature distribution of the hot blocks.

Mixed Convection Modeling. Correlations, developed on the basis of the mixed convection data described above, will be installed in the RELAP5 code.

RCCS Free Convection Modeling. Correlations, developed on the basis of the data recorded in the ANL RCCS facility, will be installed into RELAP5 for use when the cavity is modeled using RELAP5 in the future.

Multi-Species Diffusion. The two-species diffusion model incorporated in the code will be extended to a multi-species model to enable modeling the effects of air ingress during DCC events. Such events may be accompanied by graphite oxidation and the release of CO and CO_2 as well as other gases.

IHX. The NGNP system model will require a model for the IHX, which couples the coolant system to the hydrogen production system. By FY-09, sufficient information should be available to enable incorporating a mathematical model of the IHX into the code. While it is not expected to be necessary to include a mechanistic model of the hydrogen production system (it can be represented in the RELAP5/ATHENA model through the use of control blocks), it will be necessary to model the heat exchanger's heat transfer characteristics.

RELAP5/Fission Product Transport Model. The DCC event provides an opportunity for the release of fission products into the confinement/containment. The release from the fuel (including dust in the case of the pebble bed reactor), transport within the coolant system and confinement, and the deposition of these products must be calculable. To provide these capabilities, the inherent models in PARFUME (fission product release) will be augmented by the capabilities of a code such as VICTORIA. These codes will be linked to RELAP5/ATHENA in FY-10 using the existing PVMEXEC protocol.

6.6.2 Coupled Code Development Activities

Coupled code development activities are centered on enabling multiple CFD sessions to be coupled to a systems analysis model (concurrent Fluent models), coupling the RELAP5 neutronics model (NESTLE) to CFD software, coupling the PEBBED neutronics code to RELAP5, and coupling a fission product transport model (Victoria) to RELAP5.

Concurrent Fluent Models. A coupled RELAP5/Fluent model will be used to model the reactor vessel for the PCC events, in which Fluent will model the inlet and outlet plena and RELAP5/ATHENA will model the core region. To accomplish this, the present capability to link RELAP5/ATHENA models to Fluent models must be extended to enable concurrent Fluent models communicating with the RELAP5/ATHENA model.

Neutronics. It may be desirable to model part of the core region (prismatic or pebble bed) using Fluent, and the remainder with RELAP5/ATHENA. This would enable a direct comparison of coolant channel flow behavior between the codes under the same conditions. However, the current RELAP5/Fluent coupling protocol does not allow neutronic information to be exchanged between the codes.

RELAP5/PEBBED. PEBBED will be the neutronic module for the pebble bed reactor. It is proposed to link PEBBED with RELAP5/ATHENA in FY-08, assuming a pebble bed design has been chosen by then. The linkage strategy will be the same as that currently employed with the NESTLE code.

Coupling Fission Product Transport Software to RELAP5. This task couples the fission product transport code Victoria to RELAP5.

6.6.3 CFD Development

CFD development plans are based on the methodology described in Figure 25. Hence, there are three tracks. Track 1 is followed when a validation is performed on a commercial CFD code such as Fluent and the validation is shown to be reasonable. Thus, the commercial CFD code is shown to be adequate for performing certain types of calculations. Track 2 is followed when CFD code development is required—and either the source code of a commercial CFD code is used as the basis for development or the source code of a national laboratory source code is developed. Finally, Track 3 represents a separate parallel track where new CFD codes are needed to specifically address the complex simulation needs of the NGNP. The efforts to develop new CFD codes will be guided by the need for increased efficiency and accuracy using advanced numerical methods not available in existing codes or new numerical methods that have significant promise. It is anticipated that extensive CFD development will be required, particularly since the lower plenum has a large array of turbulence scales and thus will probably not be well-calculated using RANS models. Hence, LES and/or DNS will likely be required.

6.6.4 Summary

The timeline of the development activities is given in Figure 36. The total estimated cost for the development effort is $4,500k.

6.6.5 Thermal-Hydraulics R&D: Step vi—Analyses

Four analyses are planned on the basis of need. A hot channel analysis and a set of lower plenum mixing analyses are planned using a CFD code while a core heat transfer analysis and a bypass analysis are planned using RELAP5. In addition, analysis activities are required to maintain an up-to-date model of the NGNP that corresponds to the various phases of the vendor design: pre-conceptual, conceptual, preliminary, and final. It is envisioned that various calculations will be performed as the NGNP is being designed to gain a better understanding of the system behavior and to also produce alternate results that can be used to confirm the expected behavior of the NGNP during various operational conditions or accident scenarios.

Hot Channel Analyses. Circumferential and radial variation of the heat generation rate in the core causes nonuniform heating in the coolant channels during normal operations. The temperature of the helium in the hottest cooling channel must be accurately estimated to determine the worst environment that will be seen by the associated materials, especially in the lower plenum and the exit duct. The temperature at the exits of the cooling channels will also provide inlet conditions for modeling the flow in the lower plenum. In essence the task is designed to obtain the “best-estimate” calculation of the helium exit temperature from the “hot” channel, as identified by the highest local peaking factors for a typical prismatic reactor design for the conditions identified in Table 2. The Fluent CFD code is the tool that will be used to perform this evaluation.

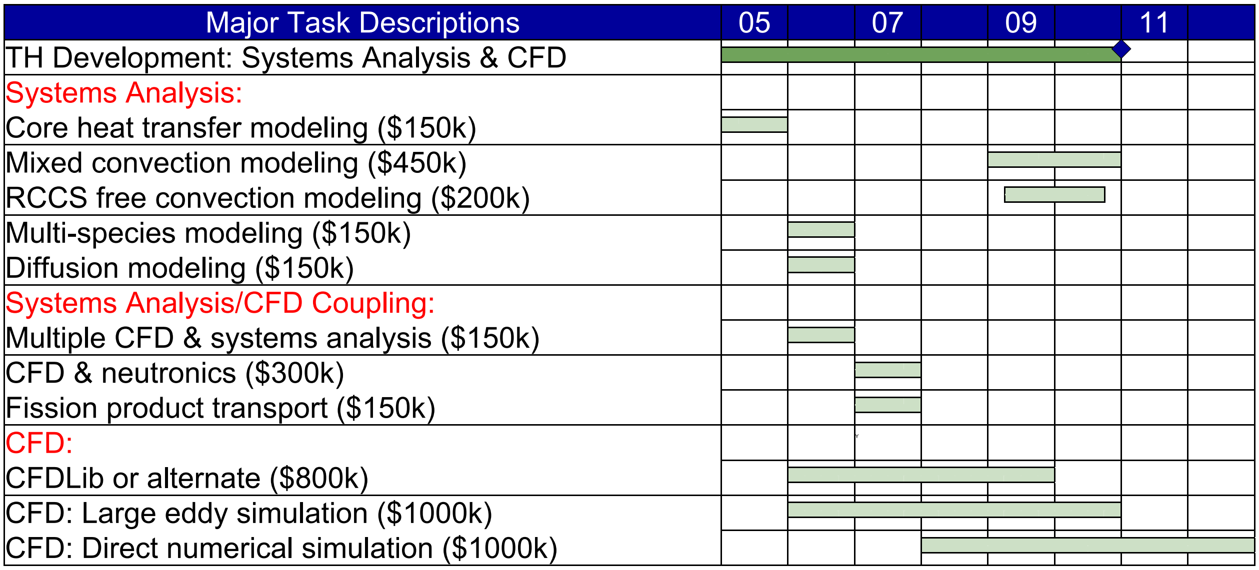

Figure 36. Timeline for thermal-hydraulic development: systems analysis & CFD codes.

Lower Plenum Mixing Analyses. Once a turbulence model has been identified that provides reasonable calculated behavior of the mixing in the lower plenum (on the basis of validation), an analysis of the lower plenum mixing and whether or not hot streaking is sufficiently large that the IHX or turbine inlet blades are threatened.

Bypass. Studies will be performed to examine the effect of a wide range in bypass on the overall performance characteristics of the NGNP.

Core Heat Transfer. Calculations will be performed to study the peak temperatures experienced in the core during the most challenging scenarios.

System Behavior Calculations. NGNP system behavior will be calculated using a systems analysis code model of the plant. The first model of the plant will be built after completion of the pre-conceptual design. Thereafter, the model will be updated during the conceptual, preliminary, and final design stages.

Summary of Analyses. The timeline of the analysis effort is given in Figure 37. The total cost (estimated) of the analysis effort is $2,330k.

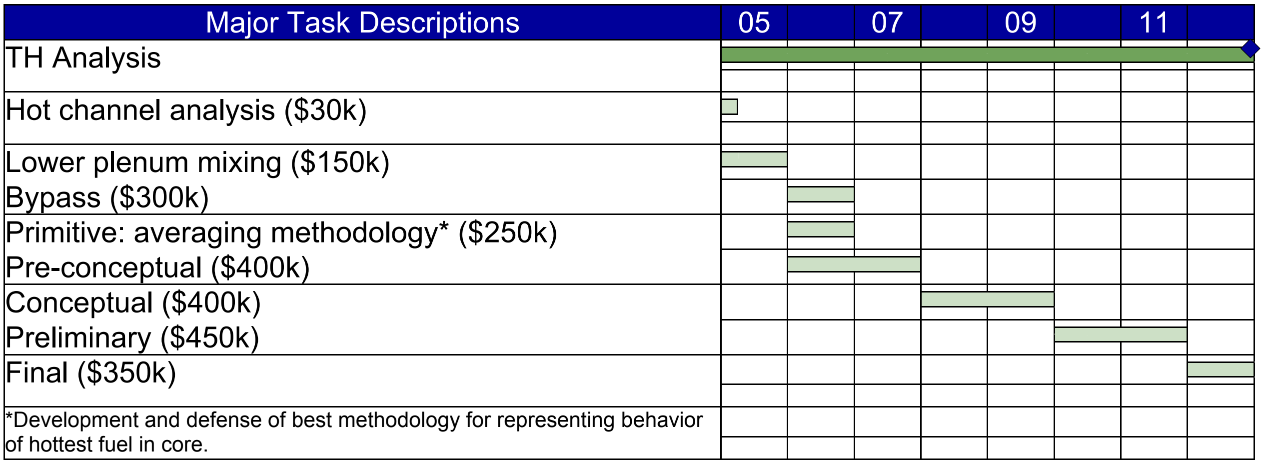

Figure 37. Timeline of thermal-hydraulic analysis effort.

7. SUMMARY

R&D projects have been initiated to ensure that the software identified in Figure 8 are validated for the DCC and PCC scenarios and the key phenomena in these scenarios that define the NGNP operational and accident envelope. The ongoing and proposed R&D are based on known requirements that stem from the "first-cut" PIRT as determined using the engineering judgment of the advanced gas-cooled reactor community. Over the next year or so, as first the NGNP Project Integrator is selected and finally the NGNP vendor is selected the reactor design will be clarified. At that point a design-specific PIRT can be defined. In the interim, the R&D requirements will continue to be expanded to include what are perceived as scenarios that are important, but of lesser importance, than the DCC, PCC, and rated operational conditions. Scenarios that fall in this category are some of the reactivity scenarios, e.g., rod ejection (Morris, Petti, Powers, and Boyack 2004).

Summary of R&D Projects[a]: Planned for immediate future or ongoing.

Region of System	Operational Conditions	Depressurized Conduction Cooldown	Pressurized Conduction Cooldown
Inlet Plenum			*IP1: Validation of CFD mixing calculation during transient.*
Core	*CO1: Nuclear data measurements to reduce calculational uncertainty.* *CO2: Modification of cross-section generation code to treat low-energy resonances with upscattering. Development of improved method for computing Dancoff factors.* **CO3: Characterization of hot channel temperatures and fluid behavior at operational conditions.** *CO4: Validation using integral experimental data.* *CO5: Additional physics modeling code improvements.*	CD1: Validation of systems analysis codes to demonstrate capability to predict thermal behavior. *CD2: Validation of models that calculate fission product release from fuel.* *CD3: Validation and calculation of air ingress and potential water ingress behavior into reactor vessel and core region.*	CP1: Validation of systems analysis codes to demonstrate capability to predict thermal and hydraulic behavior.
Outlet Plenum	PO1: Validation of CFD mixing using mixed index refraction (MIR) facility data & data available in literature	*PD1: Validation of CFD mixing during operational transients and effect on turbine operational characteristics.*	*PP1: Validation of CFD mixing during operational transients and effect on turbine operational characteristics.*
RCCS	*RO1: Validation of natural convection characteristics in cavity at operational conditions.* *RO2: Characterization of natural convection characteristics in cavity at operational conditions.*	*RD1: Validation of heat transfer & convection cooling phenomena present in reactor cavity and via RCCS.*	*RP1: Validation of heat transfer & convection cooling phenomena present in reactor cavity and via RCCS.*
Turbine Inlet	*TO1: Validation of CFD mixing between outlet plenum and turbine inlet; effect of temperature variation on turbine blade thermal stresses*		
Downcomer & Vessel Structure		VD1: Validation of peak vessel wall temperatures as predicted using CFD.	VP1: Validation of peak vessel wall temperatures as predicted using CFD.
Containment		*ConD1: Validation of fission product transport, including dust, into containment and regions for potential release to environment.*	
System Behavior	SO1: Validation & calculation of system operational envelope—including turbine/compressor components.	SD1: Validation & calculation of reactor systems.	SP1: Validation & calculation of reactor systems.

a. **Bold black font = ongoing work**; normal font = some work completed but more proposed; *italic font = proposed work.*

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